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A

# A Generalization of the Method of Conjugate Gradients for Solving Systems of Linear Algebraic Equations

It is the purpose of this note to establish a slight generalization of the method of conjugate gradients for solving linear equations. The generalization will then be used to provide a unified theory for two rather different algorithms which have been proposed for the case in which the matrix of the equations is not symmetric. The corresponding formulas for the determinant of the matrix will also be developed, although they are probably without much practical interest.

We shall use capital letters for matrices, Greek letters for vectors, and lower case Roman letters for scalars. All matrices will be real and of order $n \times n$, and all vectors will be real and of dimensionality $n$. We denote the transpose of a matrix or a vector by a prime.

Let $S$ be a positive definite matrix. The method[1] of conjugate gradients is based upon the construction of two sequences of vectors $\gamma_0, \gamma_1, \cdots$ and $\delta_0, \delta_1, \cdots$, and a sequence of scalars $a_0, a_1, \cdots$. The sequences are constructed by repeated substitution into the following formulas:

$$\gamma_0 = \delta_0, \tag{1}$$

$$a_N = \frac{\gamma_N' \gamma_N}{\delta_N' S \delta_N}, \quad N = 0, 1, \cdots, n-1, \tag{2}$$

$$\gamma_{N+1} = \gamma_N - a_N S \delta_N, \quad N = 0, 1, \cdots, n-1, \tag{3}$$

$$b_N = \frac{\gamma'_{N+1} \gamma_{N+1}}{\gamma_N' \gamma_N}, \quad N = 0, 1, \cdots, n-2, \tag{4}$$

$$\delta_{N+1} = \gamma_{N+1} + b_N \delta_N, \quad N = 0, 1, \cdots, n-2. \tag{5}$$

To avoid discussing exceptional cases, we adopt the convention that if $\delta_N = 0$ for some value of $N$, say $N = N_0$, then $\delta_{N_0+1}, \cdots, \delta_{n-1}$ and $\gamma_{N_0+1}, \cdots, \gamma_n$ are to be defined as being zero vectors.

HESTENES & STIEFEL[1] proved a long series of interesting results concerning the sequence of vectors generated by (1)–(5). In particular, they showed that the vectors $\gamma_0, \gamma_1, \cdots, \gamma_{n-1}$ are orthogonal (or zero) and the vectors $\delta_0, \delta_1, \cdots, \delta_{n-1}$ are $S$-orthogonal or conjugate with respect to $S$. Moreover, they show that the scalars $a_N$ given by (2) are identical with the coefficients in the representation of $\gamma_0$ by a linear combination of the vectors $S\delta_N$. That is,

$$\gamma_0 = \sum_0^{n-1} a_k S \delta_k. \tag{6}$$

From this it can be deduced that the two quadratic forms $\gamma_N' S^{-1}\gamma_N$ and $(S^{-1}\gamma_N)'(S^{-1}\gamma_N)$ are reduced in value at each step.

Hestenes & Stiefel also mention without a specific proof that $\det S = (a_0 a_1 \cdots a_{n-1})^{-1}$, where $\det S$ stands for the determinant of $S$. This relation is valid only if $\gamma_0$ and $S$ are such that $\delta_N \neq 0$, $N \leqq n-1$. A proof of this relation can be given as follows: Let $\Delta$ be the matrix whose columns are $\delta_0, \cdots, \delta_{n-1}$, and let $G$ be the matrix whose columns are $\gamma_0, \cdots, \gamma_{n-1}$. Then by the $S$-orthogonality of the vectors $\delta_N$, it follows that $\Delta' S\Delta = D$, where $D$ is a principal diagonal matrix whose principal diagonal elements are $\delta_0' S\delta_0$, $\delta_1' S\delta_1, \cdots, \delta_{n-1}' S\delta_{n-1}$. But from (5) it is seen that $\delta_N$ is the sum of $\gamma_N$ and a linear combination of the vectors $\gamma_0, \gamma_1, \cdots, \gamma_{N-1}$. Therefore by an elementary property of determinants, $\det \Delta = \det G$. Since the vectors $\gamma_N$ are orthogonal, $G'G$ is a principal diagonal matrix whose diagonal elements are $\gamma_0'\gamma_0, \gamma_1'\gamma_1, \cdots, \gamma_{n-1}'\gamma_{n-1}$. Putting these facts together, we get

$$\det S = \frac{\det D}{\det \Delta' \det \Delta} = \frac{\det D}{\det \Delta' \Delta} = \frac{\det D}{\det G'G} = \prod_{k=0}^{n-1} \frac{\delta_k' S\delta_k}{\gamma_k'\gamma_k} = \frac{1}{a_0 a_1 \cdots a_{n-1}}. \tag{7}$$

We now consider the applicability of the construction given by (1)–(5) to the problem $A\xi = \eta$, where $A$ is an arbitrary non-singular matrix, $\eta$ is a given vector, and $\xi$ is an unknown vector.

Choose an initial estimate $\xi_0$ of the solution $A^{-1}\eta$ of $A\xi = \eta$. Choose any positive definite $S$. Let $B$ be an arbitrary non-singular matrix. Construct the sequences given by the algorithm with $\gamma_0 = \delta_0 = B(\eta - A\xi_0)$. Then by (6)

$$B(\eta - A\xi_0) = \sum_0^{n-1} a_k S\delta_k,$$

or

$$A^{-1}\eta = \xi_0 + \sum_0^{n-1} a_k A^{-1}B^{-1}S\delta_k.$$

To apply this result, it is advantageous to express $S$ in the form

$$S = BATA'B',$$

where $T$ is a positive definite matrix. Then the solution of $A^{-1}\eta$ is given by

$$A^{-1}\eta = \xi_0 + \sum_{k=0}^{n-1} a_k TA'B'\delta_k.$$

The solution can be expressed iteratively, if desired, by the recursion relation

$$\xi_{N+1} = \xi_N + a_N TA'B'\delta_N, \quad N = 0, \cdots, n-1. \tag{9}$$

From (7), we see that the absolute value of the determinant of $A$ is given by

$$|\det A| = \frac{1}{(a_0 a_1 \cdots a_{n-1} \det T)^{\frac{1}{2}} |\det B|}.$$

For some purposes it might be convenient to rewrite the relevant parts of the algorithms (1)–(6) in terms of the residual vectors $\zeta_N = \eta - A\xi_N$. To do this we notice that (9) and (3) imply that

$$B(\eta - A\xi_N) = B\rho_N = B\rho_0 - \sum_{k=0}^{N-1} a_k BATA'B'\delta_k = \gamma_N.$$

Thus we have only to replace $\gamma_N$ by $B\rho_N$ in (1)–(5) to obtain the desired modification. The new relations are

(1)′ $$\delta_0 = B\rho_0,$$

(2)′ $$a_N = \frac{(B\rho_N)'B\rho_N}{\delta_N'BATA'B'\delta_N}, \quad N = 0, \cdots, n-1,$$

(3)′ $$\rho_{N+1} = \rho_N - a_N ATA'B'\delta_N, \quad N = 0, \cdots, n-1,$$

(4)′ $$b_N = \frac{(B\rho_{N+1})'B\rho_{N+1}}{(B\rho_N)'B\rho_N}, \quad N = 0, \cdots, n-2,$$

(5)′ $$\delta_{N+1} = B\rho_{N+1} + b_N\delta_N, \quad N = 0, \cdots, n-2.$$

These formulas, together with (9), represent the generalization of the conjugate gradient algorithm for the problem $A\xi = \eta$ which was promised in the first paragraph.

We shall now specialize $T$ and $B$ so as to obtain algorithms useful in practice.

*Case 1.* $B = I$, $T = A^{-1}$, $A$ positive definite. The algorithm (1)′–(5)′, (9), assumes the standard fundamental form given by Hestenes & Stiefel.[1]

*Case 2.* $B = A'$, $T = (A'A)^{-1}$. The formulas (1)′–(5)′ become:

$$\delta_0 = A'\rho_0,$$

$$a_N = \frac{(A'\rho_N)'A'\rho_N}{(A\rho_N)'(A\rho_N)}, \quad N = 0, \cdots, n-1,$$

$$\rho_{N+1} = \rho_N - a_N A\delta_N, \quad N = 0, \cdots, n-1,$$

$$b_N = \frac{(A'\rho_{N+1})'A\rho_{N+1}}{(A'\rho_N)'A\rho_N}, \quad N = 0, \cdots, n-2,$$

$$\delta_{N+1} = A'\rho_{N+1} + b_N\delta_N, \quad N = 0, \cdots, n-2.$$

The iterations (9) for the solution vector $\xi = A^{-1}\eta$ are given by

$$\xi_{N+1} = \xi_N + a_N\delta_N, \quad N = 0, \cdots, n-1,$$

and

$$|\det A| = (a_0 a_1 \cdots a_{n-1})^{-\frac{1}{2}}.$$

This is the method of solution for the case of an arbitrary non-singular $A$ proposed by Hestenes & Stiefel.[1] The algorithm constructs a set of $A'A$-orthogonal vectors $\delta_N$.

*Case 3.* $B = I$, $T = I$. The formulas (1)′–(5)′ or (1)–(5) (there is no difference in this case) become:

$$\delta_0 = \rho_0,$$

$$a_N = \frac{\rho_N{}'\rho_N}{\delta_N{}'AA'\delta_N}, \quad N = 0, \cdots, n-1,$$

$$\rho_{N+1} = \rho_N - a_N AA'\delta_N, \quad N = 0, \cdots, n-1,$$

$$b_N = \frac{\rho_{N+1}{}'\rho_{N+1}}{\rho_N{}'\rho_N}, \quad N = 0, \cdots, n-2,$$

$$\delta_{N+1} = \rho_{N+1} + b_N\delta_N, \quad N = 0, \cdots, n-2.$$

The iterations for the solution vector $\xi = A^{-1}\eta$ are given by

$$\xi_{N+1} = \xi_N + a_N A'\delta_N, \quad N = 0, \cdots, n-1.$$

The formula for the determinant is again

$$|\det A| = (a_0\, a_1 \cdots a_{n-1})^{-1}.$$

The algorithm constructs a set of $AA'$-orthogonal vectors $\delta_N$ instead of a set of $A'A$-orthogonal vectors, as in Case 2.

This method of solution for the case of an arbitrary non-singular A was proposed by CRAIG.[2] The author learned of this method through a communication from Dr. Craig dated May 22, 1953, in which an algorithm essentially equivalent to the one given above was stated, but with $\rho_N$ calculated at each step from the relation $\rho_N = \eta - A\xi_N$. It has an obvious advantage over the Hestenes-Stiefel proposal in that the number of arithmetic operations required is slightly smaller.

To be specific, if we measure the amount of computing work only by the required number of multiplications, assuming no zero elements, and counting a division as two multiplications, the count for the first step of the Craig method is $3n^2 + 5n + 4$, whereas that for the Hestenes-Stiefel method is $4n^2 + 6n + 4$. The detailed breakdown is as follows. First, for the Craig method, $\rho_0$ is $n^2$ multiplications, $A'\delta_0$ is then $n^2$, $a_0$ is $2n + 2$, $\xi_1$ is $n$, $\rho_1$ is $n^2$, $\rho_1{}'\rho_1$ is $n$, $b_0$ is 2 (we already have computed $\rho_0{}'\rho_0$ for $a_0$), $\delta_1$ is $n$; total $3n^2 + 5n + 4$. With the Hestenes-Steifel method, $\rho_0$ is $n^2$, $\delta_0$ is $n^2$, $A\delta_0$ is $n^2$, $a_0$ is $2n + 2$, $\xi_1$ is $n$, $\rho_1$ is $n$ (it is true that we already have computed $A\delta_0$, but not $a_0A\rho_0$ nor $Aa_0\delta_0$), $A'\rho_1$ is $n^2$, $(A'\rho_1)'A'\rho_1$ is $n$, $b_1$ is 2, $\delta_1$ is $n$; total $4n^2 + 6n + 4$. We are obviously assuming full storage of all vectors computed in the previous step at each point in the computation. The detailed breakdown is given here because the author has encountered a number of apparent discrepancies in similar counts published elsewhere (not necessarily relating to the methods discussed here); these discrepancies doubtless arise largely from different orderings of operations and different assumptions as to what will be stored after computation.

After the first step there is little to choose between the two methods from the standpoint of the number of multiplications theoretically required. In the Craig method, each step after the first and before the last takes $2n^2 + 4n + 4$.

In the Hestenes-Stiefel method, the corresponding count is $2n^2 + 5n + 4$. In the latter method, if $\rho_n$ in the last step were to be computed from the recursion relation, the method would win back the $n^2$ multiplications which it lost to the Craig method in the first step; but it would hardly be reasonable to calculate the last residual in this way.

We note that since the algorithm in either case will very probably last for $n$ steps unless a peculiarly fortunate choice of $\xi_0$ was made, the total number of multiplications to be expected is of the order of $2n^3$. The eventual justification for the use of conjugate gradient methods in preference to the most economical direct methods (which theoretically require only $n^3/3 + O(n^2)$ multiplications) must rest on definitive *a priori* studies of round-off error, and on the peculiarities of individual computing machines, and on special characteristics of the matrix $A$. But it seems quite probable at this writing that no final recommendations will ever be formulated as to the "best" ways of solving linear equations.

There is a further practical use for the algorithm (1)′–(5)′ other than the applications represented by the specializations described above. It may be possible under some circumstances to find a matrix $B$ such that premultiplication of the equation $A\xi = \eta$ by $B$ will improve the "condition"[3] of $A$. Then (1)′–(5)′, with $T$ chosen conveniently, say $T = (A'A)^{-1}$, might give an advantageous algorithm to use. (With $T = (A'A)^{-1}$ the algorithm would be the same as that of Case 2 but with $A$ replaced by $B'$.)

In conclusion, we note that Hestenes & Stiefel[1] assert (p. 424–425) that the most general cg-algorithm for any linear system is obtained from (1)′–(5)′ by assuming that $BA$ is positive definite and $T = (A'B')^{-1}$. Nevertheless without this specialization, the generality of (1)′–(5)′ seems to exceed the limits specified by Hestenes & Stiefel, because here $B$ is an arbitrary non-singular matrix. The disagreement, if it may be called that, seems to lie in the fact that their characterization of generality is derived from a certain generalization of the method of conjugate directions, and this generalization does not include all the possibilities represented by the algorithm given here.

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[1] M. R. HESTENES & E. STIEFEL, "Methods of conjugate gradients for solving linear systems," NBS *Jn. of Research*, v. 49, 1952, p. 409–436.
[2] E. J. CRAIG, *Iteration Procedures for Simultaneous Equations*. Doctoral dissertation, Mass. Inst. Tech., Cambridge, Mass., 1954.
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# On the Estimation of Quadrature Errors for Analytic Functions

**1. Introduction.** The present paper sets forth a complex variable method for the estimation of errors which arise when approximate rules of quadrature are applied to analytic functions. In contrast to the usual real variable methods, this method does not involve the use of the higher derivatives of the function, but uses only a knowledge of the size of the function in the complex plane. It is therefore of practical value when dealing with situations

in which the higher derivatives of the function are difficult to obtain in closed form, or where the higher derivatives become excessively large over the interval in question.

The principal feature of this method is the use of the characteristic inequality for bounded linear functionals. The method was developed substantially in DAVIS[2] and outlined there not only for quadratures but also for rules of differentiation, interpolation, etc. Numerical coefficients were obtained for several rules for the case of functions analytic in the unit circle. In the present paper, we consider only quadrature formulas. We deal with certain commonly applied rules of low order and also some Gaussian rules of rather high order, and present a table of coefficients (Table 2) which permits the rapid estimation of errors (through formulas (26), (31), (38)) when these rules are applied to functions which are analytic on a closed interval $[a,b]$. The estimates given here provide upper bounds for the error and their use leads to a conservative practice. In a certain sense, as will be explained in § 4, these estimates are best possible. The problem of obtaining very precise estimates of error is a difficult one and such estimates can be obtained only after a painstaking analysis of the particular function integrated. When estimates are developed which are applicable to wide classes of functions, some precision is necessarily lost. It is felt that the present method provides a compromise between the time involved in making the estimate and the precision of the estimate. It should be added that in any case, the precision of the present estimates is independent of the precision of conventional estimates obtained by using the maximum value of some high derivative over the integration interval; that is, for some functions the former will provide the sharper estimate while for other functions the latter will.

The consideration of classes of functions which are analytic on a closed interval (as opposed to functions which are analytic in a fixed circle) provides more freedom with but slightly more work. This freedom shows up particularly when dealing with functions which are analytic on the segment of integration but which have singularities within the circle constructed on this segment as a diameter. Functions which are analytic on the interval of integration are most conveniently handled by the introduction of the Chebyshev polynomials. These polynomials are orthogonal (with respect to a weight) not only over the real interval but over certain ellipses in the complex plane, and the resulting complex analytic Fourier analysis lends considerable simplicity to the developments which follow.

We reiterate that we are dealing with functions which are analytic on a closed line segment and hence are continuable analytically to some two dimensional region of the complex plane which contains that segment in its interior. Thus, we rule out the cases where the function to be integrated has only low order continuity properties or the case where the function has been extracted from an ensemble of functions with only certain statistical facts known.

**2. The Class $L^2(\mathcal{E}_\rho)$.** Let $B$ designate a bounded region lying in the plane of the complex variable $z = x + iy$. By $L^2(B)$, we shall mean the class of functions which are single-valued regular analytic in $B$ and are such that

$$\iint_B |f(z)|^2 dxdy < \infty. \tag{1}$$

The class $L^2(B)$ has been studied extensively. For the fundamentals of this theory see BERGMAN.[1] We note in particular that if $f(z)$ is regular in the closure of $B$, then (1) holds. The positive square root of the quantity (1) is generally termed the *norm* of $f$ over $L^2(B)$ and is designated by $\|f\|$ or $\|f\|_B$. That is,

$$\|f\|_B = \left( \iint_B |f(z)|^2 dxdy \right)^{\frac{1}{2}}; \quad f \epsilon L^2(B). \tag{2}$$

If a region $G$ satisfies $G \subseteq B$ and if $f \epsilon L^2(B)$, it is clear that $f \epsilon L^2(G)$ and that

$$\|f\|_G \leq \|f\|_B. \tag{3}$$

The principal features of the class $L^2(B)$ are as follows. We introduce the integral

$$\iint_B f(z)\overline{g(z)}dxdy = (f,g); \quad f, g \epsilon L^2(B), \tag{4}$$

as an inner product. The class $L^2(B)$ possesses complete orthonormal systems $\{\zeta_n(z)\}$ in the sense of (4). Every function of the class can be expanded in a Fourier series

$$f(z) = \sum_{n=0}^{\infty} a_n \zeta_n(z), \tag{5}$$

wherein

$$a_n = (f, \zeta_n) \quad (n = 0,1,\cdots). \tag{6}$$

The convergence of (5) is uniform and absolute in every closed subregion of $B$. Moreover, we have

$$\|f\|^2 = \sum_{n=0}^{\infty} |a_n|^2. \tag{7}$$

The bilinear series $\sum_{n=0}^{\infty} \zeta_n(z)\overline{\zeta_n(w)}$ converges for $z, w \epsilon B$ to a function $K_B(z,\bar{w})$, generally designated as the Bergman kernel function of $B$, which posseses the characteristic reproducing property, $(f(z), K_B(z,\bar{w})) = f(w)$ for all $f \epsilon L^2(B)$. For simply connected regions $B$ with a Jordan boundary, there exists a complete orthonormal set of polynomials $\{p_n(z)\}$.

There are, moreover, two notable cases wherein the polynomials $p_n(z)$ have a particularly simple structure. They are the circle and the ellipse. The circle $|z| < R$ possesses the set of polynomials

$$p_n(z) = (n+1)^{\frac{1}{2}} \pi^{-\frac{1}{2}} z^n R^{-n-1} \quad (n = 0,1,\cdots) \tag{8}$$

as a complete orthonormal system.

To discuss the case of the ellipse, it is best to assume that it has been placed in a normalized position. Let an ellipse, therefore, have its major axis along the $x$ axis and its foci at the points $(-1,0)$ and $(1,0)$. Let $a$ and $b = (a^2 - 1)^{\frac{1}{2}}$ designate its semimajor and semiminor axes respectively and let

the quantity $\rho = \rho(a)$ be defined by

$$\rho = (a + b)^2, \quad a = \tfrac{1}{2}(\rho^{\frac{1}{2}} + \rho^{-\frac{1}{2}}), \quad b = \tfrac{1}{2}(\rho^{\frac{1}{2}} - \rho^{-\frac{1}{2}}). \tag{9}$$

This ellipse will be designated by $\mathcal{E}_\rho$. For values of $\rho > 1$, these ellipses form a confocal family and collapse to the segment $[-1, +1]$ as $\rho \to 1$. In Table 1 will be found the values of the geometric quantities $b$ and $\rho$ for a number of selected values of $a$.

We introduce the Chebyshev polynomials of the second kind by means of the definition

$$U_n(z) = (1 - z^2)^{-\frac{1}{2}} \sin((n + 1) \arccos z) \quad (n = 0,1,\cdots). \tag{10}$$

It can then be shown that the polynomials

$$\zeta_n(z) = 2(n + 1)^{\frac{1}{2}}\pi^{-\frac{1}{2}}(\rho^{n+1} - \rho^{-n-1})^{-\frac{1}{2}}U_n(z), \quad (n = 0,1,\cdots) \tag{11}$$

form a complete orthonormal system for $L^2(\mathcal{E}_\rho)$.

**3. Quadrature Errors for $L^2(\mathcal{E}_\rho)$.** In conformity with the above normalization, we shall assume that the integration to be performed is over the interval $[-1, 1]$. The case of an arbitrary interval may be handled by means of an appropriate linear transformation [see § 6]. An arbitrary $N + 1$ point quadrature formula is given by

$$\int_{-1}^{+1} f(x)dx \sim \sum_{k=0}^{N} a_k f(\lambda_k) \equiv R(f) \tag{12}$$

where $\lambda_k$ are certain abscissas lying in $[-1,1]$ and $a_k$ are the associated weights. The error $E \equiv E(f)$ involved in the rule $R$ is

$$E(f) = \int_{-1}^{1} f(x)dx - R(f) \tag{13}$$

and may be regarded as a linear functional on $f$.

If $f(x)$ is analytic on $[-1,1]$ then it is clear that for some value of $\rho > 1$, $f$ may be continued analytically so as to be regular in the closed ellipse $\bar{\mathcal{E}}_\rho$. Such an $f(z)$ is therefore of class $L^2(\mathcal{E}_\rho)$, and may be expanded in a series of Chebyshev polynomials,

$$f(z) = \sum_{n=0}^{\infty} a_n\zeta_n(z); \quad \sum_{n=0}^{\infty} |a_n|^2 = \|f\|^2 < \infty, \tag{14}$$

which converges uniformly and absolutely in the interior of $\mathcal{E}_\rho$. Applying the operator $E$ to (14) we obtain

$$E(f) = \sum_{n=0}^{\infty} a_n E(\zeta_n). \tag{15}$$

Estimating $E(f)$ by means of the Schwarz inequality, there is obtained

$$|E(f)|^2 \leq \sum_{n=0}^{\infty} |a_n|^2 \sum_{n=0}^{\infty} |E(\zeta_n)|^2. \tag{16}$$

Let us now write

$$\sigma^2 = \sigma_R^2 = \sum_{n=0}^{\infty} |E(\zeta_n)|^2; \tag{17}$$

then in view of (7) there is obtained

$$|E(f)| \leq \sigma_R \|f\|. \tag{18}$$

The quantity $\sigma_R$ which is the norm over $L^2(\mathcal{E}_\rho)$ of the bounded linear functional $E$ has an alternate representation in the form $\sigma_R^2 = E_z E_{\bar{w}} K_R(z,\bar{w})$. It therefore depends only upon the ellipse $\mathcal{E}_\rho$, and the quadrature rule $R$, but is independent of $f$ and of the particular complete orthonormal set of functions used in the expansion (14). The quantity $\sigma_R$ may therefore be computed once for all. Using (17) and (11) we have

$$\sigma_R^2 = \frac{4}{\pi} \sum_{n=0}^{\infty} (n+1) \frac{|E(U_n(z))|^2}{\rho^{n+1} - \rho^{-n-1}}. \tag{19}$$

We have, moreover,

$$U_n(z) = (n+1)^{-1} T'_{n+1}(z) \quad (n = 0,1,\cdots), \tag{20}$$

where $T_n(z)$ designates the Chebyshev polynomials of the first kind defined by

$$T_n(z) = \cos(n \arccos z) \quad (n = 0,1,\cdots). \tag{21}$$

Therefore,

$$\int_{-1}^{+1} U_n(x)dx = \frac{1}{n+1}[T_{n+1}(1) - T_{n+1}(-1)] = \frac{1}{n+1}[1 + (-1)^n]. \tag{22}$$

If quantities $\tau_n$ are defined by

$$\tau_n = 0 \qquad n \text{ odd}, \tag{23}$$

$$\tau_n = \frac{2}{n+1} \qquad n \text{ even},$$

then we have

$$\sigma_R^2 = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(n+1)}{\rho^{n+1} - \rho^{-n-1}} \left( \tau_n - \sum_{k=0}^{N} a_k U_n(\lambda_k) \right)^2. \tag{24}$$

Table 2 lists the values of $\sigma$ corresponding to the trapezoidal, Simpson's, Weddle's and the Gaussian 2,3,7,10 and 16-point formulas [For the abscissas and weights of these Gaussian rules see LOWAN[4]], and for a range of values of the parameter $\rho$. These values were computed from (24) on the National Bureau of Standards Eastern Automatic Computer (SEAC).

**4. On the Error Estimate (18).** The inequality (18) allows us to estimate quadrature errors from a table of values of $\sigma$ and from an estimate of the norm $\|f\|$. Let us assume that we are dealing with a fixed rule $R$ with error $E$. The value of the parameter $\rho$ is at our disposal to a certain extent. For func-

tions $f(x)$ which are analytic on $[-1,1]$ there will be a range of values of $\rho$, $1 < \rho < \rho^* \leq \infty$ for which $f(z) \epsilon L^2(\mathcal{E}_\rho)$. For each such $\rho$, the inequality (18) is valid. To exhibit the dependence of (18) upon $\rho$, we should write

$$|E(f)| \leq \sigma_R(\rho) \|f\|_{\mathcal{E}_\rho}, \quad 1 < \rho < \rho^*. \tag{18'}$$

Now $\|f\|_{\mathcal{E}_\rho} = 0$ when $\rho = 1$ and increases as $\rho$ increases. On the other hand $\sigma_R(\rho)$ decreases as $\rho$ increases. Hence, the best estimate will occur for some intermediate value of $\rho$. The inequality (18′) can therefore be improved by writing

$$|E(f)| \leq \min_{1<\rho<\rho^*} \sigma_R(\rho) \|f\|_{\mathcal{E}_\rho}. \tag{25}$$

Let the rule $R$ as well as the ellipse $\mathcal{E}_\rho$ be fixed. Then the inequality (18′) (which is the characteristic inequality for bounded linear functionals) is a best possible one in the following sense: there exist functions $g$ of class $L^2(\mathcal{E}_\rho)$ such that

$$|E(g)| = \sigma_R(\rho) \|g\|_{\mathcal{E}_\rho}. \tag{26}$$

In general, of course, the error will be less. There are two additional facts which in the practical carrying out of this method tend to diminish the precision of the method. The first is that the exact minimum in (25) is difficult to ascertain and what one does is simply to take the minimum of a finite number of such values. The second is that the norm of $f$ cannot be computed exactly except in the simplest cases and an appropriate upper bound must be used. The net effect of all this is to replace the right hand side of (25) with a less precise upper bound, but one which is much more readily ascertained.

**5. Methods for Estimating $\|f\|$.** It appears, then, that the principal task confronting the numerical analyst when using the present method is that of estimating the norm $\|f\|$ over some ellipse $\mathcal{E}_\rho$. In the present section we shall explain a number of devices which may be useful for this purpose. By the very definition (2) we have

$$\|f\|_{\mathcal{E}_\rho}^2 = \iint_{\mathcal{E}_\rho} |f(z)|^2 dxdy, \tag{27}$$

and it may be possible in certain simple cases to evaluate (27) directly. If $f(z)$ is continuous in the closed ellipse $\bar{\mathcal{E}}_\rho$, and if we set

$$M_\rho = \max_{z \epsilon \bar{\mathcal{E}}_\rho} |f(z)|, \tag{28}$$

then we have from (27),

$$\|f\|_{\mathcal{E}_\rho}^2 \leq M_\rho^2 \iint_{\mathcal{E}_\rho} dxdy, \tag{29}$$

so that

$$\|f\|_{\mathcal{E}_\rho} \leq \sqrt{\pi ab}\, M_\rho, \tag{30}$$

where the quantities $a$ and $b$ are related to $\rho$ by means of (9). The quantity $M_\rho$ or an upper bound for it can, in many cases, be obtained by algebraic manipulation. It may be more convenient to replace $\mathcal{E}_\rho$ by some circle containing it, say the circle $C_a$:

$$|z| \leq a = \frac{\rho + 1}{2\rho^{\frac{1}{2}}}.$$

We then have

$$\|f\|_{\mathcal{E}_\rho} < \|f\|_{C_a} \leq a\sqrt{\pi} \max_{|z| \leq a} |f(z)|, \tag{31}$$

assuming that $f(z)$ is regular in $\bar{C}_a$.

If $f(z)$ is of class $L^2(C_a)$ and its Taylor expansion is known:

$$f(z) = \sum_{n=0}^{\infty} \alpha_n z^n, \tag{32}$$

then it follows from (7) and (8) that we have

$$\|f\|^2_{C_a} = \pi a^2 \sum_{n=0}^{\infty} \frac{\alpha_n^2 a^{2n}}{n+1} \tag{33}$$

which is an exact evaluation of the middle term of the inequality (31). The quantity $\|f\|_{\mathcal{E}_\rho}$ may itself be expressed as an infinite series involving the Taylor coefficients $\alpha_n$, but such expressions are more cumbersome and consequently less useful.

It should be pointed out that in cases of great complexity, there is always the possibility of obtaining $M_\rho$ directly by evaluating $|f(z)|$ along the boundary of $\mathcal{E}_\rho$ on a sufficiently dense set of points. Despite the loss of accuracy involved in combining (18) and (30), errors obtained in this way will, in general, be better than those obtained by using the conventional real variable error expressions and estimating the derivatives which occur there by means of Cauchy's inequality. This can be explained by the fact that the real variable expressions must be valid for a wider class of functions.

**6. The Case of an Arbitrary Interval.** The quantities of Tables 1 and 2 refer to the interval $[-1,1]$. The case of an arbitrary interval $[a,b]$ is dealt with by means of the linear transformation

$$\begin{cases} x = \dfrac{2w}{b-a} - \dfrac{b+a}{b-a} \\ w = \dfrac{b-a}{2}\, x + \dfrac{b+a}{2} \end{cases} \tag{32}$$

which carries the interval $a \leq w \leq b$ into $-1 \leq x \leq 1$. Let the rule $E^*$ be given on $[a,b]$ as follows:

$$E^*(f) = \int_a^b f(w)dw - \sum_{k=0}^{N} a_k f(\lambda_k). \tag{33}$$

The analogous rule on $[-1,1]$ is given by

$$E(f) = \int_{-1}^{+1} f(x)dx - \sum_{k=0}^{N} \left(\frac{2}{b-a}\right) a_k f\left[\left(\frac{2\lambda_k}{b-a}\right) - \left(\frac{b+a}{b-a}\right)\right] \tag{34}$$

TABLE I: *Geometric Quantities for Ellipses*

| $a$ | $b$ | $\rho$ | $(\pi ab)^{\frac{1}{2}}$ |
|---|---|---|---|
| 1.01 | .1418 | 1.3266 | .6607 |
| 1.02 | .2010 | 1.4908 | .8026 |
| 1.03 | .2468 | 1.6302 | .8936 |
| 1.04 | .2857 | 1.7574 | .9661 |
| 1.05 | .3202 | 1.8773 | 1.0277 |
| 1.10 | .4583 | 2.4282 | 1.2584 |
| 1.15 | .5679 | 2.9511 | 1.4324 |
| 1.20 | .6633 | 3.4720 | 1.5814 |
| 1.25 | .7500 | 4.0000 | 1.7162 |
| 1.30 | .8307 | 4.5397 | 1.8420 |
| 1.40 | .9798 | 5.6634 | 2.0759 |
| 1.50 | 1.1180 | 6.8541 | 2.2953 |
| 1.75 | 1.4361 | 10.1515 | 2.8099 |
| 2.00 | 1.7321 | 13.9282 | 3.2989 |
| 2.50 | 2.2913 | 22.9565 | 4.2421 |
| 3.00 | 2.8284 | 33.9706 | 5.1631 |
| 4.00 | 3.8730 | 61.9839 | 6.9763 |
| 5.00 | 4.8990 | 97.9898 | 8.7723 |

and is known by the same name. If $f(w)$ is analytic on $[a,b]$, then

$$g(x) = f\left[\left(\frac{b-a}{2}\right)x + \frac{b+a}{2}\right] \tag{35}$$

is analytic on $[-1,1]$ and, setting $x_k = \dfrac{2\lambda_k}{b-a} - \dfrac{b+a}{b-a}$, we have

$$E^*(f) = \int_a^b f(w)dw - \sum_{k=0}^{N} a_k f(\lambda_k) = \frac{b-a}{2}\left[\int_{-1}^{+1} g(x)dx - \sum_{k=0}^{N} a_k g(x_k)\left(\frac{2}{b-a}\right)\right], \tag{36}$$

so that from (36), (35), and (34),

$$E^*(f) = \left(\frac{b-a}{2}\right)E(g). \tag{37}$$

Thus,

$$|E^*(f)| = \frac{b-a}{2}|E(g)| \leq \left(\frac{b-a}{2}\right)\sigma_R(\rho)\|g\|_{\varepsilon_\rho}. \tag{38}$$

The $\sigma_R(\rho)$ are the tabulated values [Table 2] in the $z = x + iy$ plane and $\|g\|_{\varepsilon_\rho}$ also refers to this plane.

**7. Examples.**

1. Estimate the error $E$ incurred in evaluating $\int_0^1 \exp(e^x)dx$ by Weddle's rule. From (35) we have $g(z) = \exp(e^{(z+1)/2})$ which is an entire

TABLE 2: *Values of* $\sigma_R$

| $a$ \ $R$ | Trapezoidal | Simpson's | Weddle's | Gauss 2 pt. | Gauss 3 pt. | Gauss 7 pt. | Gauss 10 pt. | Gauss 16 pt. |
|---|---|---|---|---|---|---|---|---|
| 1.01 | 1.216 ( 1) | 4.048 ( 0) | 1.237 ( 0) | 1.184 ( 0) | 9.512 (−1) | 4.060 (− 1) | 2.050 (− 1) | 4.737 (− 2) |
| 1.02 | 6.007 ( 0) | 1.995 ( 0) | 5.835 (−1) | 7.710 (−1) | 5.790 (−1) | 1.670 (− 1) | 5.997 (− 2) | 6.900 (− 3) |
| 1.03 | 3.962 ( 0) | 1.309 ( 0) | 3.585 (−1) | 5.834 (−1) | 4.109 (−1) | 8.521 (− 2) | 2.346 (− 2) | 1.580 (− 3) |
| 1.04 | 2.941 ( 0) | 9.632 (−1) | 2.449 (−1) | 4.696 (−1) | 3.115 (−1) | 4.846 (− 2) | 1.066 (− 2) | 4.572 (− 4) |
| 1.05 | 2.329 ( 0) | 7.550 (−1) | 1.774 (−1) | 3.912 (−1) | 2.453 (−1) | 2.952 (− 2) | 5.236 (− 3) | 1.538 (− 4) |
| 1.1 | 1.110 ( 0) | 3.339 (−1) | 5.318 (−2) | 1.989 (−1) | 9.843 (−2) | 4.284 (− 3) | 3.573 (− 4) | 2.197 (− 6) |
| 1.15 | 7.064 (−1) | 1.935 (−1) | 2.181 (−2) | 1.211 (−1) | 4.959 (−2) | 9.913 (− 4) | 4.608 (− 5) | 8.820 (− 7) |
| 1.2 | 5.059 (−1) | 1.255 (−1) | 1.045 (−2) | 8.033 (−2) | 2.805 (−2) | 2.931 (− 4) | 8.363 (− 6) | 6.037 (− 9) |
| 1.25 | 3.865 (−1) | 8.682 (−2) | 5.518 (−3) | 5.628 (−2) | 1.708 (−2) | 1.015 (− 4) | 1.829 (− 6) | 5.644 (−10) |
| 1.3 | 3.075 (−1) | 6.272 (−2) | 3.125 (−3) | 4.097 (−2) | 1.097 (−2) | 3.933 (− 5) | 5.007 (− 7) | 7.234 (−11) |
| 1.4 | 2.105 (−1) | 3.574 (−2) | 1.162 (−3) | 2.355 (−2) | 5.054 (−3) | 7.475 (− 6) | 4.909 (− 8) | 1.882 (−12) |
| 1.5 | 1.539 (−1) | 2.208 (−2) | 4.969 (−4) | 1.461 (−2) | 2.592 (−3) | 1.812 (− 6) | 6.620 (− 9) | 8.074 (−14) |
| 1.75 | 8.271 (−2) | 8.228 (−3) | 8.824 (−5) | 5.467 (−3) | 6.553 (−4) | 9.380 (− 8) | 1.071 (−10) | 1.238 (−16) |
| 2.0 | 5.084 (−2) | 3.725 (−3) | 2.237 (−5) | 2.479 (−3) | 2.166 (−4) | 8.749 (− 9) | 3.869 (−12) | 6.699 (−19) |
| 2.5 | 2.382 (−2) | 1.067 (−3) | 2.836 (−6) | 7.107 (−4) | 3.768 (−5) | 2.063 (−10) | 2.037 (−14) | 1.760 (−21) |
| 3.0 | 1.320 (−2) | 4.002 (−4) | 6.064 (−7) | 2.668 (−4) | 9.558 (−6) | 1.092 (−11) | 3.325 (−16) | 2.736 (−25) |
| 4.0 | 5.344 (−3) | 8.896 (−5) | 6.443 (−8) | 5.899 (−5) | 1.165 (−6) | 1.200 (−13) | 6.018 (−19) | 1.342 (−29) |
| 5.0 | 2.688 (−3) | 2.822 (−5) | 1.244 (−8) | 1.908 (−5) | 2.345 (−7) | 3.867 (−15) | 4.909 (−21) | 7.011 (−33) |

Values in the parentheses indicate the power of 10 by which the tabulated values should be multiplied.

function of $z$ and is therefore of class $L^2(\mathcal{E}_\rho)$ for all $\rho > 1$. Now, $|\exp(e^{(z+1)/2})| = \exp[\mathrm{Re}(e^{(z+1)/2})] = \exp[e^{(x+1)/2}\cos y/2]$. Thus on $\mathcal{E}_\rho$ we have $|\exp(e^{(z+1)/2})| \leq \exp[e^{(a+1)/2}]$. By (38) and (30) we have

$$|E| < \tfrac{1}{2}(\pi ab)^{\frac{1}{2}} \exp[e^{(a+1)/2}]\sigma_w. \tag{39}$$

According to (18′), the estimate (39) is valid for all $a > 1$. Of the values tabulated, the right member of (39) is minimized for $a = 2.5$ and yields

$$|E| < \tfrac{1}{2}(4.242)(315.7)(2.836 \times 10^{-6}) \doteq .0019. \tag{40}$$

In the above work, the norm of $\exp(e^{(z+1)/2})$ has been estimated crudely, and a number of improvements suggest themselves. Thus, for instance, $|\exp(e^{(z+1)/2})| < \exp(e^{(x+1)/2})$, and since this last function is concave upward, we have

$$\exp(e^{(x+1)/2}) \leq \tfrac{1}{2}[\exp(e^{(a+1)/2}) + \exp(e^{(-a+1)/2})] + \frac{x}{2a}[\exp e^{(a+1)/2}) - \exp(e^{(-a+1)/2})], \quad -a \leq x \leq a. \tag{41}$$

It is now easily verified that for arbitrary $A,B,C$,

$$\iint_{\mathcal{E}_\rho} (Ax + By + C)^2 dxdy = \pi ab\left(\frac{A^2a^2}{4} + \frac{B^2b^2}{4} + C^2\right), \tag{42}$$

so that we have

$$|E| < \tfrac{1}{2}(\pi ab)^{\frac{1}{2}}\left(\frac{A^2a^2}{4} + C^2\right)^{\frac{1}{2}}\sigma_w \tag{43}$$

where

$$A = \frac{1}{2a}[\exp(e^{(a+1)/2}) - \exp(e^{(-a+1)/2})], \tag{44}$$

$$C = \tfrac{1}{2}[\exp(e^{(a+1)/2} + \exp(e^{(-a+1)/2})].$$

For $a = 2.5$, we have $A = 162.82$, $C = 158.65$, so that

$$|E| < \tfrac{1}{2}(4.2421)(160.6)(2.836 \times 10^{-6}) = .00097 \tag{45}$$

A conventional estimate of error using the formula

$$|E| \leq \max_{0\leq\xi\leq 1}\left[\frac{h^7}{140}f^{(6)}(\xi) + \frac{9h^9}{1400}f^{(8)}(\xi)\right]; \quad f(x) = \exp(e^x),$$

yielded the value $|E| \leq .006$.

2. Estimate the error $E$ incurred in evaluating $\int_2^4 \Gamma(w)dw$ by means of the 7-point Gaussian rule. This is a case where conventional methods cannot be used due to the lack of information about the higher derivatives of the integrand. Transferring to the interval $[-1,1]$ we must consider the function $g(z) = \Gamma(\frac{1}{2}(z+7))$. This function is regular in $|z| < 7$; hence we may take $a$ in the range $1 < a < 7$. Now,[5] $|\Gamma(x+iy)| \leq \Gamma(x)$ for $x > 0$

so that $|g(z)| = |\Gamma(\frac{1}{2}(x+7)+\frac{1}{2}iy)| \leq \Gamma[\frac{1}{2}(x+7)]$. By the concavity of the $\Gamma$ function, $|g(z)| \leq \max\{\Gamma(\frac{1}{2}(a+7)), \Gamma(\frac{1}{2}(-a+7))\}$, $z \epsilon \mathcal{E}_\rho$. Thus we have from (38) and (30),

$$|E| < \tfrac{1}{2}(\pi ab)^{\frac{1}{2}} \max\{\Gamma(\tfrac{1}{2}(a+7)), \Gamma(\tfrac{1}{2}(-a+7))\}\, \sigma_{G_7(a)}. \tag{46}$$

The selection $a = 5.0$ yields

$$|E| \leq \tfrac{1}{2}(8.772)(120)(3.867 \times 10^{-15}) \doteq 2.04 \times 10^{-12}. \tag{47}$$

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# Integrals Occurring in Problems of Molecular Structure

In theoretical work on molecular structure based either upon the valence bond method or upon the molecular orbital method, the electronic wave functions are usually built up from atomic orbitals (AO's). The calculation of most physical and chemical quantities then reduces to the evaluation of a number of integrals involving these orbitals. It is customary to adopt SLATER[1] type AO's, defined by (cf. RÜDENBERG[2])

$$\begin{aligned}
(1s) &= (\zeta^3/\pi)^{\frac{1}{2}}e^{-\zeta r} & (3d\bar{\pi}) &= (2\zeta^7/3\pi)^{\frac{1}{2}}yze^{-\zeta r}\\
(2s) &= (\zeta^5/\pi)^{\frac{1}{2}}re^{-\zeta r} & (3s) &= (2\zeta^7/5\pi)^{\frac{1}{2}}(r^2/3)^{-\zeta r}\\
(2p\sigma) &= (\zeta^5/\pi)^{\frac{1}{2}}ze^{-\zeta r} & (3p\sigma) &= (2\zeta^7/15\pi)^{\frac{1}{2}}zre^{-\zeta r}\\
(2p\pi) &= (\zeta^5/\pi)^{\frac{1}{2}}xe^{-\zeta r} & (3p\pi) &= (2\zeta^7/15\pi)^{\frac{1}{2}}xre^{-\zeta r}\\
(2p\bar{\pi}) &= (\zeta^5/\pi)^{\frac{1}{2}}ye^{-\zeta r} & (3p\bar{\pi}) &= (2\zeta^7/15\pi)^{\frac{1}{2}}yre^{-\zeta r}\\
(3d\sigma) &= (\zeta^7/2\pi)^{\frac{1}{2}}(z^2 - r^2/3)e^{-\zeta r} & (3d\delta) &= (2\zeta^7/3\pi)^{\frac{1}{2}}\tfrac{1}{2}(x^2 - y^2)e^{-\zeta r}\\
(3d\pi) &= (2\zeta^7/3\pi)^{\frac{1}{2}}xze^{-\zeta r} & (3d\bar{\delta}) &= (2\zeta^7/3\pi)^{\frac{1}{2}}xye^{-\zeta r}
\end{aligned}$$

where $(x,y,z)$ are the cartesian coordinates of the electron referred to the nucleus as origin with the $z$-axis directed along the internuclear axis towards the other nucleus, $r^2 = x^2 + y^2 + z^2$ and $\zeta$ is a numerical screening parameter. Occasionally complex Slater type AO's are used; however since these are simply linear combinations of the real Slater AO's, no distinction will be made between integrals involving real and complex orbitals.

Of the distinct types of two-centre integrals that arise, six are of major

importance; if $\chi_a$, $\chi_{a'}$ etc. denote orbitals of nucleus $a$ and $\chi_b$, $\chi_{b'}$ etc. orbitals of nucleus $b$, these are*

Overlap integrals:

$$(\chi_a|\chi_b) = \int \chi_a\chi_b\, dv.$$

Direct Coulomb attraction integrals:

$$(\chi_a|1/r_b|\chi_a) = \int \chi_a(1/r_b)\chi_a\, dv.$$

Exchange Coulomb attraction integrals:

$$(\chi_a|1/r_b|\chi_b) = \int \chi_a(1/r_b)\chi_b\, dv.$$

Coulomb repulsion integrals:

$$(\chi_a\chi_b|\chi_{a'}\chi_{b'}) = \int\int \chi_a(1)\chi_b(2)(1/r_{12})\chi_{a'}(1)\chi_{b'}(2)dv_1dv_2.$$

Hybrid or ionic integrals:

$$(\chi_a\chi_{a'}|\chi_{a''}\chi_b) = \int\int \chi_a(1)\chi_{a'}(2)(1/r_{12})\chi_{a''}(1)\chi_b(2)dv_1dv_2.$$

Exchange integrals:

$$(\chi_a\chi_b|\chi_{b'}\chi_{a'}) = \int\int \chi_a(1)\chi_b(2)(1/r_{12})\chi_{b'}(1)\chi_{a'}(2)dv_1dv_2.$$

in which $r_b$ is the distance of the electron from nucleus $b$, (1) and (2) represent all the coordinates of electrons 1 and 2 respectively and $r_{12}$ is the distance between these electrons. The internuclear distance $R$ enters all the integrals as a parameter.

There are essentially only two methods of evaluating such integrals, one of which consists of using expansions of the reciprocals of the electron distances and the other expansions of the orbitals. The first method is based upon the pioneer work of SUGIURA,[3] ZENER & GUILLEMIN,[4] BARTLETT,[5] ROSEN,[6] JAMES[7] and others whilst the second is largely due to BARNETT & COULSON[8] following a suggestion by COOLIDGE.[9] The choice of method for any particular problem is somewhat arbitrary and will probably be decided in the future by the availability of suitable tables.

The first method as used in the past has necessitated the computation of a large number of auxiliary integrals, defined as follows:

$$A_n(x) = \int_1^\infty e^{-xt}\, t^n\, dt; \quad B_n(x) = \int_{-1}^{+1} e^{-xt}\, t^n\, dt;$$

$$G_\tau^{\nu}(n;x) = \int_{-1}^{+1} e^{-xt}\, P_\tau^{\nu}(t) t^m (1 - t^2)^{\nu/2} dt,$$

where $P_\tau^{\nu}(t)$ is the associated Legendre function of the first kind[10];

$$f_\tau(m;x) = \int_1^\infty Q_\tau(t) e^{-xt}\, t^m\, dt,$$

where $Q_\tau^\nu(t)$ is the associated Legendre function of the second kind;[10]

$$F_{k,m,n}(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t^2-1)^k(t+t')^{-(k+1)}t^m t'^n e^{-xt}e^{-yt'};$$

$$J_n(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t^2-1)(1-t'^2)(t^2-t'^2)(t+t')^n e^{-xt}e^{-yt'};$$

$$K_n(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t^2-1)(1-t'^2)(1+tt')^2(t+t')^{n-2}e^{-xt}e^{-yt'};$$

$$F_{m,n}(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t+t')^{-m}(-t')^n(1-t'^2)^{m-1}e^{-xt}e^{-yt'};$$

$$S_\tau(m,n;x) = \int_1^\infty dtQ_\tau(t)\, e^{-xt}\, t^m\, dt \int_1^t e^{-xt'}\, t'^n\, dt';$$

$$\sigma_\tau(m,n;x) = \int_1^\infty dtQ_\tau(t)\, e^{-xt}\, t^m\, dt \int_t^\infty e^{-xt'}\, t'^n\, dt';$$

$$H_\tau(m,n;x) = S_\tau(m,n;x) + S_\tau(n,m;x);$$

$$W_\tau^\nu(m,n;x) = \int_1^\infty dt \int_1^\infty dt' Q_\tau^\nu(t>)P_\tau^\nu(t<)e^{-x(t+t')}t^m t'^n(t'^2-1)^{\nu/2}.$$

All of these auxiliary integrals are expressable in terms of polynomials, exponentials, natural logarithms and the exponential integral $-\mathrm{Ei}(-x) = \int_x^\infty t^{-1}e^{-t}dt$. Many of them are simply related to each other. There is a distressing lack of uniformity not only in the choice of auxiliary integrals computed but also in the notation.

The second method, which is particularly valuable in the case of integrals involving more than two centres, requires the computation of certain so-called $\zeta$-functions which are expressable ultimately in terms of Bessel functions of half-integral orders for which the argument is pure imaginary.[11]

Several approximations to the exchange and hybrid two-centre integrals and to multi-centred integrals have been suggested[12] and their accuracy has recently been assessed by comparison with the exact values[13].

This review concludes with three bibliographies;

A—Reduction of two-centre molecular integrals

B—Tables of two-centre molecular integrals

C—Multi-centre integrals.

A very large number of papers relevant to molecular integrals has been published and it is not possible (nor desirable) to describe all of them. Bibliography A is a somewhat arbitrary selection of papers chosen so that any integral that has been calculated to date may be found in at least one of them and chosen to include also those papers which the reviewer considers to be the most useful. Bibliography B describes in as much detail as space allows the tables of two-centre integrals and of auxiliary functions which

have been published since the date of inception of *MTAC* in 1943. Excluded from this bibliography is the multitude of published material which contains only a few isolated integrals and whose usefulness is effectively restricted to the problem concerned in the particular reference. Warning must be given that owing to the complexity of the work, the occurrence of errors is frequent, even the corrections being by no means exhaustive or completely reliable. The final bibliography C lists without description (apart from title) those papers concerned with multi-centre integrals. No systematic tabulation of multi-centre integrals has yet been published.

Information on tables published prior to 1943 may be obtained from the FMR *Index*[14] and from the excellent bibliographies of MULLIGAN,[15] ROOTHAAN[16] and RÜDENBERG.[17]

Finally it seems worthwhile to mention that a discussion of future developments was reported in the proceedings of a conference on quantal methods in valence theory (QMVT).[18]

## Bibliography A

*Reduction of two-centre molecular integrals.*

N. ROSEN, "Calculations of interactions between atoms with *s*-electrons," *Phys. Rev.*, v. 38, 1931, p. 255–276. Almost all types of molecular integrals involving identical *ns* orbitals.

M. KOTANI, A. AMEMIYA & T. SIMOSE, "Tables of integrals useful for the calculations of molecular energies I," Phys.-Math. Soc. Japan, *Proc.*, v. 20, 1938, Extra no. 1, p. 1–70. Most of the integrals involving $n = 2$ orbitals with a common screening parameter and a large number over 1*s* and $n = 2$ orbitals, the $n = 2$ orbitals having a common screening parameter.

C. A. COULSON, "Two-centre integrals occurring in the theory of molecular structure," Camb. Phil. Soc., *Proc.*, v. 38, 1941, p. 210–223. A wide selection of one electron integrals over *ns* and $np\sigma$ orbitals with no restriction on the screening parameters.

R. G. PARR & B. L. CRAWFORD, JR., "On certain integrals useful in molecular orbital calculations," *Jn. Chem. Phys.*, v. 16, 1948, p. 1049–1056. Most types of integrals over like $2p\pi$ orbitals.

R. S. MULLIKEN, C. A. RIEKE, D. ORLOFF & H. ORLOFF, "Formulas and numerical tables for overlap integrals," *Jn. Chem. Phys.*, v. 17, 1949, p. 1249–1267. Overlap integrals over all combinations of *ns*, $np\sigma$, and $np\pi$ AO's for $n = 1,2,3,5$ with no restriction on the screening parameters.

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# Characters of the Symmetric Groups of Degree 15 and 16

**Introduction.** The construction of the complete character table for the symmetric group of a given degree $n$ (i.e., the group formed by the permutations of $n$ quantities) is a problem of long standing. Theoretically the problem was solved many years ago by FROBENIUS,[1] who first introduced the concept of the character of a representation (thus meriting the title of founder of the theory of group representations). Frobenius' expression for the symmetric group characters as coefficients of a certain algebraic form is, however, unsuitable for practical calculation except for groups of quite low degree. Some years ago MURNAGHAN[2] was able to derive a recursion scheme which permits one to calculate the characters for a given $n$ in terms of the (presumably known) characters of all the symmetric groups of lower degree. This scheme has been employed by various authors[3] to construct character tables for all the symmetric groups of degree $n \leqslant 14$. The recursion scheme effectively reduces the problem to an exercise in bookkeeping, but, despite its simplicity, it suffers from two practical faults. First of all, the labor involved in computing the characters by hand becomes prohibitive for $n$ larger than, say, 14. Secondly, as mentioned above, for each $n$ the results for all lower $n$ must be used, so that errors may be expected to propagate. This, of course, is not a *theoretical* limitation, since in principle each table may be calculated, *ab initio*, and any given table can be checked for consistency by using the fact that the characters themselves satisfy certain orthogonality relations. The impracticability of proceeding by hand computation is clear when it is remembered that the number of characters of the symmetric group of degree $n$ is equal to the square of the number of unrestricted partitions of $n$; for $n = 15$, this number is 30,976.

It should be evident that the practical difficulties mentioned in the preceding paragraph can in large measure be overcome by the use of electronic computers. In fact, it seemed to us that this very calculation would provide a very good test of the speed and flexibility of such a computer with regard to the handling of purely algebraic problems. Accordingly, we set up and carried out the calculation of the complete character tables of the symmetric groups of degree $n = 15$ and 16 using the Los Alamos Electronic Computer (MANIAC). The method was checked by re-computing the tables[4] for $n = 10$ to $n = 14$. The method of calculation is described in Sec. (III). The experience was quite encouraging, and suggests that it would be profitable to apply electronic computer techniques to a large class of quite complicated problems in algebra and group theory.

**The Character Formulae.** For convenience we give here a brief resume of the relevant properties of the symmetric group characters. For proofs and detailed discussion the reader is referred to the standard works of LITTLEWOOD[5] and MURNAGHAN.[6]

The basic fact concerning the symmetric group of degree $n$ is that both its classes and its irreducible representations are in one-to-one correspondence with the number of unrestricted partitions of the integer $n$. More precisely, each class may be denoted by a partition of $n$ into non-negative integers:

$$(\rho) \equiv (\rho_1, \rho_2 \cdots \rho_k)$$
$$\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_k \tag{1}$$
$$\sum_{i=1}^{k} \rho_i = n$$

Similarly, each irreducible representation may be so labelled. In the sequel we shall reserve the symbol $(\rho)$ to label classes, and the symbols $(\lambda)$, $(\mu)$ to label irreducible representations. In the interest of compactness we adopt the standard convention of denoting repeated parts by a super-script; thus the partition (4,3,3,3,1,1) of 15 will be written $(4,3^3,1^2)$. With regard to the labelling of classes, this notation has a simple interpretation in terms of the one-dimensional permutation representation of the group, the class $(4,3^3,1^2)$ being that which consists of one cycle of order 4, three cycles of order 3, and two cycles of order 1. For a given irreducible representation $(\lambda)$, the character of the class $(\rho)$ (i.e., the common trace of the matrices belonging to this class and representation) will be denoted by $\chi_{(\rho)}^{(\lambda)}$. For the symmetric group, $\chi$ is always an integer, positive, negative, or zero. If we consider the partition $(\rho)$ as labelling the rows and $(\lambda)$ as labelling the columns, the quantities $\chi_{(\rho)}^{(\lambda)}$ are the elements of a matrix of degree equal to the number of partitions of $n$. The $\chi_{(\rho)}^{(\lambda)}$ satisfy the following orthogonality relations:

$$\sum_{(\rho)} h_\rho \chi_{(\rho)}^{(\lambda)} \chi_{(\rho)}^{(\mu)} = n! \delta_{\lambda\mu} \tag{2a}$$

$$\sum_{(\lambda)} \chi_{(\rho)}^{(\lambda)} \chi_{(\rho')}^{(\lambda)} = \frac{n!}{h_\rho} \delta_{\rho\rho'} \tag{2b}$$

where $h_\rho$ is the number of group elements belonging to the class $(\rho)$ and is given explicitly by

$$h_\rho = \frac{n!}{1^\alpha \alpha! \, 2^\beta \beta! \, 3^\gamma \gamma! \cdots} \tag{3}$$

$\alpha$ being the number of unary cycles in $(\rho)$, $\beta$ the number of binary cycles, etc.

For every class, the character of the irreducible representation $(n)$ (corresponding to the partition of $n$ into one part) is unity; i.e.,

$$\chi_{(\rho)}^{(n)} = 1 \quad \text{for all } (\rho) \tag{4}$$

Similarly, for every class, the character corresponding to the partition $(1^n)$ is $\pm 1$, depending on whether the class $(\rho)$ is even (i.e., has an even number of cycles of even order) or odd.

$$\begin{aligned} \chi_{(\rho)}^{(1^n)} &= +1, \quad (\rho) \text{ even} \\ \chi_{(\rho)}^{(1^n)} &= -1, \quad (\rho) \text{ odd} \end{aligned} \tag{5}$$

If we denote by $(\tilde{\lambda})$ the partition of $n$ conjugate[7] to $(\lambda)$, then for every

class, the characters of the irreducible representations corresponding to $(\bar{\lambda})$ and $(\lambda)$ are related by:

$$\chi^{(\bar{\lambda})}_{(\rho)} = \chi^{(1^n)}_{(\rho)} \cdot \chi^{(\lambda)}_{(\rho)} \tag{6}$$

The consequence of this last relation is that for each $(\rho)$ we have to calculate only slightly more than half the characters, since the character of the associated representation is either equal to, or just the negative of, the character of the given representation. If $P(n)$ denotes the total number of unrestricted partitions of $n$ and $P_s(n)$ the number of self-conjugate partitions, then the total number[8] of quantities $\chi^{(\lambda)}_{(\rho)}$ which must be calculated is just $\frac{1}{2}P(n)\,[P(n) + P_s(n)]$. For $n = 15$ this number is 15,840.

The recurrence relations for the characters referred to in the introduction may be stated in the following form:[5]

Let $(\rho')$ be a partition of the integer $(n - m)$ which differs from the partition $(\rho)$ of $n$ by the omission of a cycle of order $m$. Then

$$\chi^{(\lambda)}_{(\rho)} = \sum_{(\mu)} \pm \chi^{(\mu)}_{(\rho')} \tag{7}$$

where the partitions $(\mu)$ of $(n - m)$ run over the set

$$(\mu) = (\lambda_1 - m, \lambda_2, \cdots \lambda_k), (\lambda_1, \lambda_2 - m, \lambda_3 \cdots \lambda_k), \cdots, (\lambda_1, \lambda_2 \cdots \lambda_k - m) \tag{8}$$

The partitions (8) do not in general satisfy the conditions (1), since the parts will not necessarily be in non-ascending order or even positive. It can be shown[5,6] that the following three rules may be invoked:

1. If $(\mu)$ has all its parts in non-ascending order but the last part is negative, then the contribution $\chi^{(\mu)}$ to the sum (7) is identically zero.
2. If the $i$th part of $(\mu)$ is one less than the $i + 1$st part, $\mu_i + 1 = \mu_{i+1}$, then the corresponding contribution to (7) is identically zero.
3. $\chi^{(\mu')} = -\chi^{(\mu'')}$ where $(\mu'')$ is the partition obtained from $(\mu')$ by the replacements

$$\begin{aligned} \mu'_i + 1 &\to \mu''_{i+1} \\ \mu'_{i+1} - 1 &\to \mu''_i \end{aligned} \tag{9}$$

The procedure is thus to operate on the set (8) with rule 3 until either a partition satisfying (1) is obtained or the conditions of rule 1 or 2 are satisfied. (The $\pm$ sign in (7) is intended to represent possible sign changes arising from rule 3.) In conjunction with these operating rules, (7) effectively reduces the calculation of the characters of a given group to those of groups of lower degree. By iteration of this process a complete reduction can be carried out for every given $(\rho)$ until $(\rho) = (0)$. Of course no useful closed expression for this process exists. Formulae do exist[5,6] which give $\chi^{(\lambda)}_{(\rho)}$ directly in terms of the number of cycles of various orders occurring in $(\rho)$, but they become prohibitively complicated unless $(\lambda)$ has a particularly simple form. There is, however, one explicit formula, due to Frobenius, which is of use in a practical calculation, namely that which expresses the character of the identity class $(\rho) = (1^n)$ in terms of the parts of $(\lambda)$. This may be written in the form[6]

$$\chi^{(\lambda)}_{(1^n)} = \frac{n! \prod_{i<j} (l_i - l_j)}{l_1!\, l_2! \cdots l_k!} \quad (\lambda = \lambda_1, \lambda_2, \cdots, \lambda_k) \tag{10}$$

where $l_i = \lambda_i + k - i$. This gives the trace of the unit matrix in the representation $(\lambda)$ and is hence the dimension of the representation.[9]

This completes our resume of the properties of the characters of the symmetric group. Many other relations exist, but they are not of interest for our purpose.

**Calculation Scheme.** The computer first simply prepares a table of the partitions of $n$. This table is also used to designate the classes. In addition the complete character tables for the symmetric groups of degree $n \leq 4$ are stored in the computer. Their function will be described presently

The sequence of steps performed by the computer is as follows: a character is first decomposed by (7) into a sum of characters all of the same class $(\rho')$, corresponding to a group of degree $n' (< n)$. Attention is fixed on the first component. The integers describing the partition are rearranged, if necessary, in non-ascending order, with the aid of (9). Next the partition is examined to see if

(i) its value is zero (cf. rules 1 and 2, page 214). If it is so, we proceed to the next component of the decomposition; if not, we test to see if

(ii) $n' \leq 4$. If this condition is satisfied, the computer makes reference to the appropriate character table stored in the memory; if this condition is not satisfied, the computer finally determines if

(iii) $(\rho') = (1^{n'})$. If so, the character is computed by (10). If not, a further reduction by means of (7) is made and the above procedures repeated until the first component is evaluated; all members of the original decomposition are treated in turn.

Obviously, the most efficient method of utilizing (7) is to choose the reduction parameter $m$ as large as possible, and this was always done.

The instructions, or code, for the problem occupied about one-half of the 1024 locations of the electrostatic memory; numerical storage accounted for the remaining half; the partitions occupied a small fraction of the auxiliary drum memory. The computing time for the group $n = 15$ was five hours; for $n = 16$, twelve hours were necessary to compute the 27,258 distinct characters.

Obviously, the number of operations necessary to compute a character is very heavily dependent upon the structure of the partition $(\rho)$. Indeed, for the class $(\rho) = (2^8)$ six levels of branching were required to obtain the necessary reduction and the computer took thirty-seven minutes to calculate the characters for this class. In comparison only one minute was needed to compute the characters for $(\rho) = (16)$.

Although electrostatic storage limitations precluded a complete orthogonality check on the table, (2b) was used for each class separately.

The two tables of characters have been photographed on microfilm directly from the computer print-out. Each frame contains the characters of one class. These films are available in the UMT File [UMT 195].

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[1] G. FROBENIUS, Preuss. Akad., Berlin, *SitzBer.*, 1900, p. 516. A list of Frobenius' relevant papers may be found in ref. 4 or 5.

[2] F. J. MURNAGHAN, *Am. Journal of Math.*, v. 59, 1937, p. 437. See also the paper of LITTLEWOOD & RICHARDSON.[3]

[3] D. E. LITTLEWOOD & A. R. RICHARDSON, Roy. Soc., *Phil. Trans.*, v. 233A, 1934, p. 99.

[4] M. ZIA-UD-DIN, London Math. Soc. *Proc* (2), v. 39, 1935, p. 200; *ibid.*, v. 42, 1937, p. 340.

K. KONDO, *Phys. Math. Soc. Japan*, v. 22, 1940, p. 585.

[5] D. E. LITTLEWOOD: *The Theory of Group Characters*, 2nd edition. Oxford, 1950.

[6] F. J. MURNAGHAN: *The Theory of Group Representations*. Baltimore, 1938.

[7] The partition conjugate to $(\lambda)$ is obtained by interchanging rows and columns in the Ferrers-Sylvester graph of $(\lambda)$.

[8] $P_*(n) = P(n) - 2P(n-2) + 2P(n-8) - 2P(n-18) + \cdots$. This was pointed out to us in a private communication from Professor N. J. FINE.

[9] The following question is of some practical interest: given $n$, for what partition $(\lambda)$ does (9) take its largest value, and how does this value vary with $n$? The authors have been unable to find any discussion of this problem in the literature.

## RECENT MATHEMATICAL TABLES

**1234[A].**—M. LOTKIN & M. E. YOUNG, *Table of Binomial Coefficients. Exact Values*. Ballistic Research Laboratories *Memo. Report* No. 762 Aberdeen Proving Ground, 1954, 49 p., 21.6 × 27.9 cm. Mimeographed from typescript.

This table is a sequel to RMT **1123.** It gives exact values of the coefficients

$$\frac{n!}{r!(n-r)!}$$

for $r \leq (n+1)/2$ and $n = 0(1)100$, whereas the previous table rounds these values to 20 figures. This new table will be of use in studies involving congruence properties and other theoretical properties of binomial coefficients.

D. H. L.

**1235[C,D,E].**—R. A. HIRVONEN, "Nutshell tables of mathematical functions for interpolation with calculating machines," *Bull. Géod.* No. 30, 1953, p. 369–392.

The tables presented here are one page tables. Interpolation is by means of Taylor's development which the author writes in the nested form

$$f(a+th) = \{[(Dt + C)t + B]t + A\}t + f(a)$$

so that

$$A = hf'(a), \quad B = h^2f''(a)/2!, \ldots$$

The tables therefore give the functions at coarse argument intervals together with the coefficients $A,B,C,D$. The tables are as follows:

$\ln x$ for $x = 1(.02)1.6$; 10D
$e^x$ for $x = 0(.01).2$; 10D
$\sin x$ for $x = 0°(2°)90°$; 10D
$\arctan x$ for $x = 0(.02)1$; 8D.

The latter table is in decimal parts of a degree. Three special geodesic tables are used to illustrate Taylor interpolation.

D. H. L.

1236[F].—H. GUPTA, M. S. CHEEMA & O. P. GUPTA, "On Möbius Means," Panjab Univ. *Research Bulletin* No. 42, 1954, 16 p.

The table occupying all but the first page of this work was computed in order to study conjectures of V. BRUN and C. L. SIEGEL regarding the second numerical integral of the Möbius function $\mu(n)$, the multiplicative function for which

$$\mu(p^\alpha) = -[1/\alpha].$$

If we define

$$\mu_1(n) = \sum_{k=1}^{n} \mu(k) \quad \text{and} \quad \mu_2(n) = \sum_{k=1}^{n} \mu_1(k),$$

then the conjecture of Brun is that "on the average"

$$\mu_2(n-1) = -2n + 12 + \beta n^{-1}$$

where $\beta = -18$. Siegel considered the value

$$\beta = -2\pi^2/\zeta(3) = -16.42119.$$

The authors tabulate

$$F(n) = T_0(n) = n\mu_2(n-1) + 2n^2 - 12n$$

whose average value should be $\beta$, and the successive means $T_k$ defined by

$$nT_k(n) = \sum_{\nu=1}^{n} T_{k-1}(\nu)$$

for $k = 0(1)5$, $n = 1(1)750$. Exact values of $T_0(n)$ are given. The other $T$'s are given to 3D. Graphs of $T_3$, $T_4$ and $T_5$ are given. For $375 \leq n \leq 750$, $T_5(n)$ descends nearly monotonely from $-14.3$ to $-15.0$.

D. H. L.

1237[K].—J. H. CALDWELL, "Approximating to the distributions of measures of dispersion by a power of $\chi^2$," *Biometrika*, v. 40, 1953, p. 336–346.

It is assumed that all observations are from normal populations. If the measure of dispersion is $u$, then for suitably chosen $c$ and $\lambda$, $cu^\lambda$ has approximately the $\chi^2$ distribution with $\nu$ degrees of freedom. Table 1 of this paper gives values of $\nu$, $\lambda$, $\log c$ for the range and mean deviation for sample size $n$, $n = 2(1)20$ and for the first quasi-range with $n = 10(1)30$. $\nu$ is given to 2S, $\lambda$ and $\log c$ to 5S. The first quasi-range is the difference between the largest-but-one and the smallest-but-one observations in a sample of $n$. Table 2 contains the same constants for the mean of $m$ ranges $m = 2(1)5$ and $n = 2(1)10$, where $n$ is the size of each of $m$ samples. Tables 3 and 4 give the approximate upper 5% and 1% points of the ratio of maximum value to minimum value in a set of $k$ independent ranges (each range for a sample of size $n$ from the same population). Values are given to 3S for $k = 2(1)12$ and $n = 3(1)10, 12, 15, 20$. Tables 5 and 6 give to 3S approximate upper 5% and

1% points for the ratio of maximum to minimum mean deviation for $k = 2(1)12$ and $n = 3(1)10, 12, 15, 30, 20, 60, \infty$. Tables 3 through 6 are based on the approximate distribution of Table 1 and the fact that the ratio of two independent $\chi^2$'s has an F-distribution. Adequate indications of accuracy of the approximation are stated.

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**1238[K].**—E. J. GUMBEL, *Statistical Theory of Extreme Values and Some Practical Applications*. NBS Applied Math. Series, no. 33, U. S. Gov. Printing Office, Washington, 1954, viii + 51 p., 20.1 × 25.9 cm. Price 40 cents.

This booklet contains four lectures given at the Bureau of Standards which are an excellent account of the theory of extreme values and their applications by the leading expert in this field. For the exponential type of distribution law for extreme values there is tabled (p. 29) for samples of $N = 15(5)50(10)100(50)300, 400, 500, 750, 1000$, extremes, the expected mean of the reduced (standardized) extremes, the ratio of these to the population mean, their standard deviation, and the ratio of this to the population standard deviation, all to 5D. Interpolated values for the means and standard deviations for $N = 20(1)49$ to 4D are also given (p. 31), these values being obtained from an empirically established linear relationship.

C. C. C.

**1239[K].**—H. C. HAMAKER, "'Average confidence' limits for binomial probabilities," International Stat. Inst., *Review*, v. 21, 1953, p. 17–27.

Given a random sample of $n$ from a binomial population with true percentage of defectives, $p$. If $k$ items are defective, the usual upper and lower $(1 - \alpha)$ confidence limits for $p$ are computed so that

$$\Pr\{p_k' < p < p_k\} \geq 1 - \alpha, \tag{1}$$

where the equality holds for only a few isolated cases and the confidence probability is generally greater than $1 - \alpha$. The limits are computed from incomplete Beta or $F$-tables, so that the upper limit is

$$p_k = 100v_1F/(v_2 + v_1F), \tag{2}$$

where $v_1 = 2(k + 1)$ and $v_2 = 2(n - k)$ are the degrees of freedom for $F$. A similar result holds for $p_k'$.

This article shows how the confidence probability varies as $p$ changes, for $n = 25$ and $\alpha = .20$ (Figures 3A and 5B′). Another set of confidence limits is then presented for which the confidence probability is generally less than $1 - \alpha$ (Figures 3B and 5A′). In this case the upper confidence limit is simply $p_{k-1}$.

The author proposes to use as average confidence limits:

$$\begin{aligned} &p_{uk} = (p_k + p_{k-1})/2; \quad p_{lk} = (p_k' + p_{k-1}')/2 \\ &p_{u0} = 100 - p_{ln} = p_{ul}/2 = (p_1 - p_0)/4 \\ &p_{l0} = 100 - p_{un} = 0. \end{aligned} \tag{3}$$

Tables of $p_{lk}$ and $p_{uk}$ to 1D are given for $n = 5(5)30, 40, 50, 75, 100(100)500$; $\alpha = .02, .10, .20$; $k = 1(1)20$, unless $n < 20$, when $k$ goes to $n$. These confidence limits give confidence probabilities which do not fluctuate much from $1 - \alpha$; however, the confidence probability will sometimes be less than $1 - \alpha$.

It should be mentioned that SIMON[1] presents a Bayesian method of averaging the probabilities; his limits are even narrower than those in the present article. It would be desirable to compare the true confidence probabilities for various $p$, using (2), (3) and the Simon charts.

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[1] L. E. SIMON, *An Engineer's Manual of Statistical Methods*. New York, 1941.

**1240[K].**—N. L. JOHNSON, "Some notes on the application of sequential tests in the analysis of variance," *Annals Math. Stat.*, v. 24, 1953, p. 614–623.

In the analysis of variance one often desires to test a linear hypothesis in some systematic model and such hypotheses are usually composite in nature. This paper considers the applicability of certain basic work by BARNARD[1] and COX[2] in sequential tests for composite hypotheses to such cases. Such a sequential situation could be encountered if one treated the number of observations taken in each class as a random variable or if the number of classes studied in an experiment could be increased in a sequential fashion. In order to obtain a sequential test a restriction upon the manner of increasing the number of observations is needed. With such restrictions one can evolve a sequential test which is in a form similar to the usual sequential type, but the lack of adequate tables of required distributions makes it difficult to apply the theory in the general case.

As a special case illustration the author considers a random model in one-way classification, namely

$$x_{ti} = a + u_i + z_{ti}$$

in which the $u$'s are normal variables, each with 0 means and standard deviations $\sigma_R$. Here the hypothesis is concerned with the value of $\delta = \sigma^2_R/\sigma^2$. If one is interested in a sequential test based on $\delta'' > \delta' = 0$, such a test exists, but to determine appropriate intervals for the tests, values of the criteria $\underline{G}_R$ and $\overline{G}_R$ are required. With the number $n$ of groups of size $k$ as the variable, Table Ia gives values of $\underline{G}_R$ and $\overline{G}_R$ to 3D for $\delta'' = 1$, $\delta' = 0$, $\alpha = \beta = .05$ and $k = 2(1)12, 15, 20, 30, 60, \infty$ and $n = 2(1)12, 15, 20, 30, 60$. Table $I_b$ is similar but with $\alpha = \beta = .01$.

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[1] G. A. BARNARD, "The frequency justification of certain sequential tests," *Biometrika*, v. 39, 1952, p. 144–150.
[2] D. R. COX, "Sequential tests for composite hypotheses," Cambridge Philos. Soc., *Proc.* v. 48, 1952, p. 290–299.

**1241[K].**—RAND CORP., *Offset Circle Probabilities*. Santa Monica, Calif., 1953, 18 p., 16.5 × 24.1 cm.

Consider a circle of radius $r_d$ with center located a distance $D$ from the origin in the $x,y$-plane. Let $q$ represent the probability that a sample value from the normal bivariate distribution with $\mu_x = \mu_y = 0$, $\sigma_x = \sigma_y = \sigma$, $\rho = 0$ falls outside this circle. 3D values of $q$ are tabled as a function of $D/\sigma$ and $(r_d - D)/\sigma$. Here $D/\sigma = 0(.1)6(.5)10(1)20, \infty$ and $(r_d - D)/\sigma = -3.9(.1)4$. This table was obtained from an unabridged 6D table of $q$ which was computed jointly by the Institute for Numerical Analysis, National Bureau of Standards, and the RAND Corporation. Card copies or printed listings of the unabridged table may be obtained by writing to the RAND Corporation.

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**1242[K].**—S. ROSENBAUM, "Tables for a nonparametric test of dispersion," *Annals Math. Stat.*, v. 24, 1953, p. 663–668.

Given a sample of $n$ values of a continuous random variable $X$, these tables give the upper 5% and 1% points for $m,n = 1(1)50$ of the distribution of the number of values in an additional sample of $m$ values which lie outside the extreme values of the original sample. This distribution was obtained by WILKS[1] in connection with the problem of two-sided distribution-free tolerance limits. The suggested use in this paper is as a non-parametric test of dispersion, which places the emphasis on smaller values of $m$ and $n$. However, if neither the sample nor the unsampled portion of the population exceed 50, these tables can also be used to establish the level of tolerance limit provided by the extreme values of the sample.

An approximation to the distribution for large and approximately equal values of $m$ and $n$ is also obtained. Since there is an apparent discrepancy between the 5% and 1% values obtained from this limiting distribution, and the values given by WILKS[1] for $m = n = 100$ (Table II, p. 406; $n$ and N in WILKS notation), the reviewer computed exact values of the 5% and 1% points for $m = n = 10(10)200(100)900$. From these results it was noted (a) that the values given by WILKS are in error, and (b) that, while the 5% point of the limiting distribution is correct for $m = n \geq 25$ (as can be seen from the tables), the exact 1% point does not reach that of the limiting distribution until at least $m = n > 170$.

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[1] S. S. WILKS, "Statistical prediction with special reference to the problem of tolerance limits," *Ann. Math. Stat.*, v. 12, 1942, p. 400–409.

**1243[K].**—HERBERT SOLOMON, "Distribution of the measure of a random two-dimensional set," *Annals Math. Stat.*, v. 24, 1953, p. 650–656.

$N(= 1,2)$ random circles of equal radius $W$ are dropped according to a bivariate distribution with circular symmetry specified by the parameter $\sigma$ on a fixed circle of radius $T$ with an aiming point at distance $R$ from its

center. The measure of interest is the ratio of the covered area to the total area of the fixed circle. The author calculates for $N = 1$ the probability $P_C$ of getting at least $C/W$ fraction coverage for specified values of $T, R, N, \sigma$. Until now only the first two moments were known.

Fig. 1 gives for $N = 1$ the contours of equal probability $P_C = .05$ (.05).95 as a function of $R$ for given values of $W + aT$, both in $\sigma$ units. The factor $a$ is eliminated by the use of the second figure, which shows the relation between coverage 0.05 to 1.00 and the factor $a(-.1 < a < .1)$ for fixed values of the quotient $W/T = .5, .6, .75, .85, 1, 1.2, 2, 3, 5, 10, \infty$. Thus the two figures represent the probability $P_C$ of coverage $C$ for given values of $W$, $T$ and $R$ (in $\sigma$ units).

Four short tables give for $N = 2$ the lower and upper bounds $\underline{P}_C = 1 - (1 - P_C)^2$ and $\bar{P}_C = P(c_1 + c_2 \geqq C)$ to 3D. Table I holds for $W/\sigma = 1$, $T/\sigma = 1$, $R = 0$ and $C = .1(.1).9$. Tables II and III deal with median coverage for $W = T$ and $W = 2T$ respectively. Table IV holds for $W = .5T$, $C = .2$. The graphs and tables demonstrate that a realistic decision can be made without resorting to random number devices.

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**1244[K].**—G. TAGUTI, "Tables of 5% and 1% points for the Polya-Eggenberger's distribution function," Union of Japanese Scientists and Engineers, *Reports of Statistical Application Research*, v. 2, no. 1, 1952, p. 27–32.

Table I gives to 3S the minimum values of $h$ such that

$$F(k;h,d) = \sum_{n=0}^{k} (1/n!)h(h + d)\cdots(h + (n - 1)d)(1 + d)^{-(h+nd)/d}$$

is $\geq a$, where $a = .95$ or .99, $h/d = .5(.5)15, 20, 30, 60, \infty$ and $k = 1(1)25$. Table II gives to 3S the maximum values of $h^{-1}$ such that

$$F(k;h,d) \geqq a$$

where $a = .95$ or .99, $d/h = 2., 1., .5(-.1).1, .05, 0$ and $k = 25(5)40(10)60, 75, 100, 200, 500, \infty$.

The method of preparing the tables and their accuracy is not given.

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**1245[L].**—ADMIRALTY RESEARCH LABORATORY, "Tables of $f(q,\alpha)$," A.R.L./T.3/Maths. 2.7, 13 p., Teddington, Middlesex, England.

4D tables of

$$\exp\left(-\frac{q^2 + k^2}{2}\right)\left\{I_0(kq) + 2\sum_{m=1}^{\infty}\left[\frac{\Gamma(m/2 + 1)}{\Gamma(m + 1)} \times u^{m/2}{}_1F_1(m/2; m + 1; -u)\, I_m(kq)\cos m\alpha\right]\right\}$$

for $u = 0, 1, \infty$, $k = .5(.5)3$, $\alpha = 0(10°)\ 180°$, $q = 0(.2)\ q_0$ where $q_0$ varies between 2 and 6 and is so chosen that the tabulation covers in each case the whole significant range of $q$.

A. E.

1246[L].—D. R. Bates, Kathleen Ledsham & A. L. Stewart, "Wave functions of the hydrogen molecular ion," Royal Soc. London, *Phil. Trans.*, v. 246 A, 1953, p. 215–240.

When the variables are separated in the Schrödinger equation for the electronic wave functions of $H_2^+$ in elliptic coordinates, there result the two differential equations

$$\frac{d}{d\mu}\left\{(1-\mu^2)\frac{dM}{d\mu}\right\} + \left\{-A + p^2\mu^2 - \frac{m^2}{1-\mu^2}\right\} M = 0 \tag{1}$$

$$\frac{d}{d\lambda}\left\{(\lambda^2-1)\frac{d\Lambda}{d\lambda}\right\} + \left\{A + 2R\lambda - p^2\lambda^2 - \frac{m^2}{\lambda^2-1}\right\} \Lambda = 0. \tag{2}$$

In the above, $A$ is a separation constant, and

$$p^2 = -\tfrac{1}{4}R^2E, \tag{3}$$

where $R$ is the distance between the nuclei in atomic units, and $E$ is the electronic energy in Rydbergs.

Equation (1) is the familiar (oblate) spheroidal wave equation which has been studied.[1] Corresponding to a countable set of eigenvalues $A(l,m,p)$ equation (1) has a solution of the form

$$M(l,m,p;\mu) = \sum_{s=0}^{\infty}{}' f_s(l,m,p)\, P_{m+s}^m(\mu), \tag{4}$$

where $P_{m+s}^m(\mu)$ is the associated Legendre function and $s$ is either always odd, or always even. Tables of the eigenvalues $A$ and the coefficients $f_s$ have been published in [1] as functions of $p$. The authors give corresponding tables for the parameter $R$, which are presumably of direct interest to researchers in the field, and the tables are arranged in such a manner that the various *orders* of the eigenvalues are directly identified with the "united atom designations." Ten such "states" are given in the tabulation, namely

$$ns\sigma_g,\ n = 1,2,3;\quad np\sigma_u,\ n = 2,3,4;\quad 3d\sigma_g,\quad 4f\sigma_u,\quad 2p\pi_u,\ \text{and}\ \ 3d\pi_g.$$

All ten correspond to parameters $m = 0,1$; $l = 0,1,2,3$. Corresponding to these states, the authors tabulate the functions $p$, $\sigma$, $-A'$, and $-E$, for $R = 0(.2)5(.5)9$ or 10; 5D (Table 1), and the coefficients $f_s$ (Table 2). The latter are given to five significant figures for the dominant coefficients, and to six decimals (usually) for the others. According to the authors, these were obtained by interpolation from the tables in[1]. The parameters $A'$ and $\sigma$ are defined below.

The authors also tabulate eigenvalues and coefficients corresponding to equation (2). Following Jaffé,[2] the authors write

$$\Lambda(\lambda) = (\lambda^2-1)^{m/2}(\lambda+1)^{\sigma}\exp(-p\lambda)y(\zeta) \tag{5}$$

with

$$\sigma = \frac{R}{p} - m - 1; \quad \zeta = (\lambda - 1)/(\lambda + 1)$$
$$A' = A - p^2.$$

The solution is written in the form

$$y = \sum_{t=0}^{\infty} g_t \zeta^t. \tag{6}$$

The solution exists corresponding to the eigenvalues of $\sigma$, for given $p$, $m$, and $A'$. In Table 3, the authors give the coefficients $g_t$ for the same range of $R$ as in Tables 1 and 2; four decimals are given in the tabulation. The paper also contains contour diagrams of $H_2^+$, as well as some comparisons between the exact solution for certain of the wave functions and the "L.C.A.O" approximation.

For theory and some tabulation relating to the general spheroidal wave function in the more accessible publications, see also references [3,4,5].

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[1] J. A. STRATTON, P. M. MORSE, L. J. CHU & R. A. HUTNER, *Elliptic Cylinder and Spheroidal Wave Functions*. John Wiley and Sons, Inc., New York, 1941.
[2] G. JAFFÉ, *Zeit. Phys.*, v. 87, 1934, p. 535 (author's citation).
[3] A. LEITNER & R. D. SPENCE, "The oblate spheroidal wave functions," Franklin Inst., *Jn.*, v. 249, no. 4, 1950, p. 299–321.
[4] J. MEIXNER, *Lamé's Wave Functions of the Ellipsoid of Revolution*, translated by MARY L. MAHLER, NACA, June, 1944.
[5] C. J. BOUWKAMP, "On spheroidal wave functions of order zero," *Jn. Math. Physics*, v. 26, 1947, p. 79–92.

**1247[L].**—S. CHANDRASEKHAR & DONNA ELBERT, "The roots of $Y_n(\lambda\eta)\, J_n(\lambda) - J_n(\lambda\eta)\, Y_n(\lambda) = 0$," Cambridge Phil. Soc., *Proc.*, v. 50, 1954, p. 266–268.

The authors tabulate to 5D the first root, $\lambda_1$, of the equation mentioned in the title, together with 7 to 9D values of

$$J_n(\lambda_1),\ Y_n(\lambda_1),\ J_n(\lambda_1\eta),\ Y_n(\lambda_1\eta),\ \frac{2}{\pi^2\lambda_1^2}\left\{\frac{J_n^2(\lambda_1\eta)}{J_n^2(\lambda_1)} - 1\right\}$$

for $\eta = .2$, $n = 1(1)5$; $\eta = .3(.1).5$, $n = 1(1)6$; $\eta = .6$, $n = 1(1)8$; and $\eta = .8$, $n = 1(1)12$. For $\eta = .5$, $n = 1(1)6$ they also give the corresponding quantities for the second and third zeros.

A. E.

**1248[L].**—CH. VITAL DUNSKI, "Les fonctions de Bessel d'argument complexe $x\sqrt{j}$ et les fonctions de Kelvin d'ordre zéro et 1," Soc. Roy. Sci. Liége *Bull.*, v. 23, 1954, p. 52–59.

Table I gives ber $x$, bei $x$, ker $x$, kei $x$, $\mathrm{ber}_1 x$, $\mathrm{bei}_1 x$, $\mathrm{ker}_1 x$, $\mathrm{kei}_1 x$, and Table II gives the real and imaginary parts of $J_0(xi^{\frac{1}{2}})$, $H_0^{(1)}(xi^{\frac{1}{2}})$, $i^{\frac{1}{2}} J_1(xi^{\frac{1}{2}})$, $i^{\frac{1}{2}} H_1^{(1)}(xi^{\frac{1}{2}})$. Each of the two tables occupies one page. The entries have been computed, to various degrees of accuracy, from the asymptotic expansions for 25 values of $x$ ranging from 10 to 72.

A. E.

**1249[L].**—Carl-Erik Fröberg & Philip Rabinowitz, "Tables of Coulomb wave functions," NBS Report 3033, 1954, 3 + 40 p., 20.5 × 27 cm.

$F$ and $G$ being the regular and the irregular Coulomb functions as defined in RMT **982** [*MTAC*, v. 6, p. 92], in this report

$$A_0(\eta) = [(1 - e^{-2\pi\eta})/(2\pi\eta)]^{\frac{1}{2}}, \quad A_L(\eta) = \tfrac{1}{2}(L^2 + \eta^2)^{-\frac{1}{2}} A_{L-1}(\eta)$$
$$F_{L,\eta}(\rho) = A_L(\eta)\rho^{L+1} f_{L,\eta}(\rho)$$
$$G_{L,\eta}(\rho) = A_L(\eta)\rho^{L+1} g_{L,\eta}(\rho).$$

The report contains tables of $f, f', g, g'$ and of the first five "reduced" derivatives $\frac{1}{k!}\frac{\partial^k}{\partial\eta^k}$ of these quantities for $L = 0, 5$, $\eta = 1(1)10$, $\rho = 1(1)10$. For other NBS tables of Coulomb wave functions see RMT **1091** [*MTAC*, v. 7, p. 101–102]. The present table was first announced as UMT **186** [*MTAC*, v. 8, p. 97], where further details are given.

A. E.

**1250[L].**—J. M. Hammersley, "Tables of complete elliptic integrals," NBS *Jn. of Research*, v. 50, 1953, p. 43.

The functions tabulated are $K$, $E$, and $\frac{1}{2}\pi/K$. The argument used is $p = 1/k$. The tables are for $p = 1(.01)1.3(.02)2$; 10S. The last figure is doubtful.

D. H. L.

**1251[L].**—Aldo Muggia, "Sul calcolo dell' integrale di Poisson," Accad. Sci. Torino Cl. Sci. Fis. Mat. Nat., *Atti*, v. 87, 1953, p. 116–126.

5D tables of

$$A(\tau) = 2\ln\left|\sin\frac{\tau}{2}\right|, \qquad B(\tau) = \int_{-\pi}^{\tau} t\cot\frac{t}{2}\,dt$$
$$C(\tau) = -\cot\frac{\tau}{2}, \qquad D(\tau) = -\tau\cot\frac{\tau}{2} + 2\ln\left|\sin\frac{\tau}{2}\right|$$

for $\tau = -\pi$, $-3.12(.04)-.04(.01).04(.04)4.6$. The tables were computed by Lia Errera of the computing center of the Politecnico di Torino.

A. E.

**1252[L].**—Uno Olsson, "Non-circular cylindrical gears," *Acta Polytechnica*, Mechanical Engineering Series, v. 2, no. 10, Stockholm, 1953, p. 1–215.

The author not only develops the theory for the construction of different types of non-circular gears but also furnishes directions for the production of the wheels. As a by-product of the investigation, he gives the following tables:

Table I: The arc length of the hyperbola,

Table II: The arc length of the ellipse with imaginary axes or the arc length of the sinh-curve,

Table III: The arc length of the parabola,

Table IV: The arc length of the exponential curve,

Table V: The hyperbolic argument $u$ as a function of the hyperbolic amplitude $\varphi$.

Tables I and II are given for $\varphi$ (the amplitude angle) $= 0°(1°)90°$ and $\alpha$ (the eccentric angle) $= 0°(5°)90°$; Table III for $\varphi = 0°(1°)90°$ with $\Delta'_{\frac{1}{2}}$ and $\Delta_0'' + \Delta_1''$; Table IV for $\varphi = 0°(.1°)10°$, $0°(1°)90°$ and Table V for $\varphi = 0°(.1°)90°$. All tables are given for the most part for modified functions to about 5 significant figures. A short section describing the use of higher degree interpolation, necessary in the tables, is also given.

IRENE A. STEGUN

NBSCL

**1253[L].**—L. J. SLATER, "Some new results on equivalent products," Cambridge Phil. Soc., *Proc.*, v. 50, 1954, p. 394–403.

Table 1 gives values, mostly to 8D or 8S, of

$$\left[\prod_{n=1}^{\infty}(1 - aq^n)\right]^{-1}$$

for $a = -.9(.05).95$ and $q = 0(.05)1$.

Table 2 gives 8D or 8S values of the same quantity for $a = 1, q = 0(.005).89$.

The first table is stated to be accurate to 7D except where fewer figures are given, the second, to 8D. The tables were computed on the EDSAC.

A. E.

**1254[L].**—L. J. SLATER, "The evaluation of the basic confluent hypergeometric functions," Cambridge Phil. Soc., *Proc.*, v. 50, 1954, p. 404–412.

The functions discussed and tabulated in this paper are

$$(1) \qquad \sum_{n=0}^{\infty}\frac{(q^a)_n\, y^n}{(q^b)_n\,(q)_n}$$

$$(2) \qquad \sum_{n=0}^{\infty}\frac{(q^a)_n\, y^n\, q^{\frac{1}{2}n(n+1)}}{(q^b)_n\,(q)_n}$$

where

$$(q^a)_n = (1 - q^a)(1 - q^{a+1})\cdots(1 - q^{a+n-1})$$

Table 1 is of the function (2) for $a = 0(.2)2$, $b = .2(.2)1$, $q = .9$, $y = (1 - q)x = .1(.1)1$.

Table 2 is of the same function, for the same values of $a$ and $b$, and for $q = .99$, $y = .01(.01).1$.

Table 3 is of the function (1) for the same values of $a$ and $b$, and for $q = .9$, $y = .1(.1).9$.

The values are mostly given to 7 or 8S: they were computed on the EDSAC.

A. E.

**1255[L].**—ROBERT L. STERNBERG, "A general solution of the two-frequency modulation product problem. II. Tables of the functions $A_{mn}(h,k)$," *Jn. Math. Phys.*, v. 33, 1954, p. 68–79.

"The purpose of this paper is to provide tables and evaluation methods for the functions

$$A_{mn}(h,k) = (2/\pi^2)\iint_R (\cos u + k\cos v - h)\cos mu\, du\cos nv\, dv$$

for $m,n = 0,1, |h| \leq 2, 0 < k \leq 1$ where $R$ is the region defined by

$$R: \cos u + k \cos v \geq h, \quad 0 \leq u,v \leq \pi$$

and subsequently also to tabulate briefly the first six higher order functions $A_{mn}(h,k)$."

The functions arise in the problem indicated in the title and have been investigated in an earlier paper[1] where there are also further references. The tables are to 6D.

A. E.

[1] R. L. STERNBERG & H. KAUFMAN, "A general solution of the two-frequency modulation product problem. I," *Jn. Math. Phys.*, v. 32, 1953, p. 233–242.

**1256[L].**—A. WALTHER & H. UNGER, "Mathematische Zahlentafeln, numerische Untersuchung spezieller Funktionen," *Naturforschung und Medizin in Deutschland*, 1939–1946, Band 3. Angewandte Mathematik, Teil I, p. 167–183. Verlag Chemie, Weinheim, 1953.

This valuable report covers numerical tables of special functions computed in Germany during the period under review, and also analytical work of importance in connection with the numerical computation of special functions. The report consists of three parts: A. Introduction, B. Survey of developments and results, C. Bibliography. Each of parts B and C is divided in four sections: 1. elementary functions, 2. tables pertaining to astronomy and geodesy, 3. Bessel functions, 4. other higher transcendental functions. The bibliography lists some eighty items. Many of these have been published (and reviewed in *MTAC*). In the case of most of the tables which have not been published a brief description (in the style of the FMR Index) is appended.

A. E.

**1257[L].**—M. W. WILKES, "A table of Chapman's grazing incidence integral $\mathrm{Ch}(x,\chi)$," Phys. Soc. *Proc.*, v. 67 B, 1954, p. 304–309.

This table gives

$$\mathrm{Ch}(x,\chi) = x \sin \chi \int_0^x \exp\,(\chi - x \sin \chi/\sin \lambda)\, \mathrm{cosec}^2 \lambda \, d\lambda$$

to 3D for $x = 50(50)\ 500(100)1000$, $\chi = 20°(1°)\ 100°$, excluding values of $\mathrm{Ch}(x,\chi)$ which exceed 100. The table was prepared on EDSAC, using a Gauss 5-point formula repeatedly, with automatic adjustment of the length of the interval. A more complete discussion of the machine techniques used is to appear elsewhere. Various checks were applied: recalculation for $\chi = 20°, 21°, 70°$, differencing in both directions, and use of the relation

$$\mathrm{Ch}(x,\chi) + \mathrm{Ch}(x,\pi - \chi) = 2 \exp\,(\chi - x \sin \chi)\, \mathrm{Ch}(x \sin \chi, \tfrac{1}{2}\pi).$$

The values are expected to be correct to within a unit in the last place.

J. T.

## MATHEMATICAL TABLES—ERRATA

240.—T. H. BLAKESLEY, *A Table of Hyperbolic Cosines and Sines.* London Physical Soc., 1890.

"A comparison with a corrected version of a table by HAYASHI has indicated 172 errors of one to three units of the last digit, as well as the 31 errors of 5 or more final units listed below. Errors in the argument are also included in the list. In addition 180 errors of between half and one final unit were found."

| Page | Function | *For* | *Read* |
|---|---|---|---|
| 1 | arg 0.14 | 5 | 4 |
| | arg 0.18 | 4 | 8 |
| | cosh 0.43 | .0938888 | .0938833 |
| 2 | cosh 1.12 | .7005670 | .6955670 |
| | sinh 1.12 | .3642872 | .3692872 |
| | cosh 1.84 | .2276799 | .2276778 |
| 3 | cosh 2.03 | .8727101 | .8727109 |
| | sinh 2.03 | .7413746 | .7413754 |
| | cosh 2.04 | .9103184 | .9103190 |
| | sinh 2.04 | .7802896 | .7802902 |
| | cosh 2.05 | .9483548 | .9483180 |
| | sinh 2.05 | .8196198 | .8195831 |
| | cosh 2.06 | .9867111 | .9867119 |
| | sinh 2.06 | .8592571 | .8592579 |
| | cosh 2.07 | .0255038 | .0255044 |
| | sinh 2.07 | .8993179 | .8993187 |
| | cosh 2.08 | .0647395 | .0646996 |
| | sinh 2.08 | .9398093 | .9397694 |
| | cosh 2.35 | .2905196 | .2904694 |
| | sinh 2.35 | .1951504 | .1951003 |
| | cosh 2.42 | .6673910 | .6673905 |
| | sinh 2.42 | .5784683 | .5784688 |
| | cosh 2.61 | .8362940 | .8362927 |
| | sinh 2.61 | .7627595 | .7626582 |
| | cosh 2.62 | .9042644 | .9042632 |
| | sinh 2.62 | .8314615 | .8314604 |
| | cosh 2.63 | .9729254 | .9729242 |
| | sinh 2.63 | .9008469 | .9008457 |
| | cosh 2.64 | .0422838 | .0422824 |
| | sinh 2.64 | .9709225 | .9709212 |
| | cosh 2.65 | .1123463 | .1123449 |
| | sinh 2.65 | .0416950 | .0416937 |
| 4 | sinh 3.15 | .6966062 | .6466062 |
| | arg 3.84 | 3 | 4 |

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**241.**—P. C. MAHALANOBIS, "Tables of random samples from a normal population," *Sankhȳa*, v. 1, 1933, p. 303–328.

We reconstructed MAHALANOBIS' table of random normal deviates as follows: Using the random numbers from TIPPETT's table (*Tracts for Computers*, No. 15, Cambridge 1927) as probabilities, we read the corresponding, normal deviate from the *Kelley Statistical Tables* (I), New York, 1938. In doing so, we found 427 errors which are greater than 0.001, of which 219 errors are greater than 0.01 with 132 errors greater than 0.1. In addition, the rows on ten pages are in the wrong order, and some blocks of numbers are totally incorrect, and much of page 306 is repeated on page 308.

Plans are being made to publish revised tables in *Sankhȳa*.

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## UNPUBLISHED MATHEMATICAL TABLES

Unpublished tables of special functions are mentioned in RMT **1256** and in *Phil. Mag.*, s. 7, v. 45, 1954, p. 599–609.

**191[A].**—F. L. MIKSA, *A Table of Binomial Coefficients for* N = 1 *to* N = 100. Typewritten manuscript of 41 p. deposited in the UMT FILE. Other copies are obtainable gratis from the author.

This table gives exact values of the binomial coefficients for the first hundred integer powers. It is thus equivalent to RMT **1234.** A comparison of the two tables has not been made.

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**192[F].**—A. FERRIER, *Étude de* $5n^2 + 1$ *et* $5n^4 + 1$. 13 typewritten pages deposited in the UMT FILE.

This study is in three parts. The first part gives the solutions $n$ of the congruences

$$5n^2 + 1 \equiv 0 \pmod{p}, \quad p < 12000$$
$$5n^4 + 1 \equiv 0 \pmod{p}, \quad p < 12000$$

The second part is a list of numbers $5n^2 + 1$ for $n \leqslant 5000$ which have a prime factor exceeding $10^7$. The last part is a factor table of $5n^4 + 1$ complete to $n = 100$ and partially complete to $n = 1000$.

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**193[F].**—F. L. MIKSA, *Table of All Primitive Pythagorean Triangles Having Equal Areas Below* 97017 29310. Twelve mimeographed leaves deposited in the UMT FILE.

Fermat noted that if $m$ and $n$ are integers then the two triangles whose sides are equal to the absolute values of

$$(3n - m)^2n^2 + m^2(m + n)^2, \quad (3n - m)^2n^2 - m^2(m + n)^2, \quad 2mn(2mn - m^2 + 3n^2)$$

and

$$(3n + m)^2n^2 + m^2(m - n)^2, \quad (3n + m)^2n^2 - m^2(m - n)^2, \quad 2mn(2mn + m^2 - 3n^2)$$

constitute a pair of Pythagorean triangles of equal area. Not all such pairs are given by this rule, however. The table gives all pairs of such triangles which are primitive whose areas do not exceed $10^{10}$, arranged according to increasing area. Besides the area, which is given also in factored form, the three sides and the Pythagorean generators of the triangles are given. There are 149 such pairs of triangles and one triplet. Of these only 81 are given by Fermat's rule. The triplet is made up of triangles whose sides are

(8580,3059,9109) (1380,19019,19069) (5852,4485,7373)

Each has an area of 13123110.

F. L. MIKSA

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Aurora, Illinois

194[F].—F. L. MIKSA, *Counts of Primitive Pythagorean Triangles by Area.* 7 Hectographed leaves deposited in the UMT FILE.

This list gives the number of primitive Pythagorean triangles whose areas lie between various limits, up to $10^{10}$. More precisely the intervals are

$$n \cdot 10^k \leqslant A < (n + 1) \cdot 10^k$$

for

$$k = 6, \quad n = 1(1)9$$
$$k = 7, \quad n = 1(1)99$$
$$k = 8, \quad n = 10(1)99$$

The total count for triangles with area less than $10^{10}$ is 52482.

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195[G].—R. L. BIVINS, N. METROPOLIS, P. R. STEIN & M. B. WELLS, *Character Tables for Symmetric Groups of Degree* 15 *and* 16. One reel of microfilm deposited in the UMT FILE.

This table is the one referred to in the authors' paper *MTAC*, v. 8, p. 212–216.

196[K].—MARY G. NATRELLA, *Critical Values for Wilcoxon Rank Sum Test.* Six mimeographed leaves deposited in the UMT FILE.

Critical values of smaller rank sum for the Wilcoxon test for the 5,2, and 1 percent significance levels are given. These are compiled from various published tables with corrections of all known errata in the originals.

C. EISENHART

NBSSEC

197[L].—A. OPLER, *Table Related to the Error Function*. 20 leaves tabulated from punched cards deposited in the UMT FILE.

The table gives 6S values of the integral

$$2 \exp(z^2) \int_z^\infty \exp(-t^2)\, dt$$

for $z = -4.5(.1)100$, together with first differences. The table is probably good to only 5S for most of the range.

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## AUTOMATIC COMPUTING MACHINERY

Edited by the Staff of the National Applied Mathematics Laboratory of the National Bureau of Standards. Correspondence regarding the Section should be directed to Dr. E. W. CANNON, 415 South Building, National Bureau of Standards, Washington 25, D. C.

### BIBLIOGRAPHY OF CODING PROCEDURE

**68.** J. L. JONES, *A Survey of Automatic Coding Techniques for Digital Computers.*

This MIT master's thesis is one of the first publications on the general subject of automatic coding. It includes chapters on the basic forms of automatic coding, a survey of present techniques, and a survey of contemplated techniques with comments. It includes an appendix of additional applications of the interpretive method and an appendix listing computer groups interested in automatic coding.

**69.** C. C. ELGOT, U. S. Naval Ordnance Laboratory, White Oak, Md., *Single v. Triple Address Computing Machines* (NAVORD Report 2741).

By utilizing a slightly idealized notion of a single address computer, the author obtains a partial answer to the question of whether a single address or a triple address computing machine requires fewer words to specify a sequence of instructions. While he finds that fewer words are required to code by means of an "idealized" single address machine, it is interesting to note that the pseudo codes for single address machines tend to be three-address codes.

**70.** H. B. CURRY, U. S. Naval Ordnance Laboratory, White Oak, Md. *A Program Composition Technique as Applied to Inverse Interpolation* (NOL Memorandum 10337).

**71.** J. W. BACKUS, International Business Machines Corporation. Operational Characteristics of the IBM 704.

The IBM 704 differs from the 701 in that among other things four floating point operations have been added along with automatic address modification. Here floating binary point representation similar to that presently used in pseudo-codes can be utilized directly by the computer.

**72.** W. BROWN, J. DETURK, H. HARNER, E. LEWIS, University of Michigan. The MIDSAC Computer.

The MIDSAC is a high-speed digital computer designed for use in an automatic control system. This 55 page booklet includes chapters on programming rules and operational characteristics, a detailed description of the computer, and the physical construction of the computer.

**73.** G. E. FORSYTHE, SWAC *computes all* 126 *distinct semigroups of order* 4. Manuscript 5 p.

The problem of finding all (non-isomorphic) groups of a given order is known to be very difficult unless the order is of a very special nature. The possibility of using electronic computing machines in this connection has occurred to a number of people, but until now no results have appeared. An idea of the complexity of the problem is obtained from a study of this computation of all distinct semigroups of order 4. By semigroup is meant a set of elements closed under an associative composition law, called multiplication for simplicity; two such sets are distinct if they are neither isomorphic nor anti-isomorphic. (Two systems are called isomorphic (anti-isomorphic) if a one-to-one mapping $X \to X'$ exists such that $(AB)' = A'B'$ $(= B'A')$.)

For machine purposes the elements of the semigroups are denoted by 0,1,2,3. The semigroup is then completely described by its multiplication table, i.e., the matrix $(a_{ij})$, $i,j = 0,1,2,3$, where $a_{ij}$ is an integer which specifies the product of the elements $i,j$. Four SWAC codes have been prepared by Forsythe in order to make a table on punched cards of all 3492 semigroups of order 4 and to pick out the 126 distinct among them (in previous work only 121 have been found). The 4 rows of the multiplication table are listed in one line consecutively, e.g. 0000 0000 0023 0032. The distinct semigroups are represented by normal forms distinguished through lexicographic order.

The first code checks on the associativity. A direct test of all the $4^{16}$ multiplication tables would take SWAC about 13 years. However, by testing partial tables, and then rejecting blocks, the time was cut down to less than 80 minutes. The second code is for obtaining the normal form. The third code picks out the distinct semigroups. The fourth code converts the 126 tables from base 2 notation to base 4.

The codes used are on file at UCNAR and NBSCL.

OLGA TAUSSKY

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## BIBLIOGRAPHY Z

**1147.** H. J. GRAY, JR., "Numerical methods in real-time simulation," *Quart. of Applied Math.*, v. 12, 1954, p. 133–140.

Under the sponsorship of the Office of Naval Research, Special Devices Center, the University of Pennsylvania conducted a study to determine the feasibility of building a digital real-time simulator for a system described by thirteen first-order non-linear differential equations. It was found necessary to improve either the speed of the digital machine or the quality of the method of solution. The paper deals with the latter problem and especially with the buildup of errors.

The paper is introductory in nature, and only linear constant-parameter systems of ordinary differential equations are considered. The characteristic

equation associated with the corresponding difference equation is found and solved by conformal mapping. A diagram is given showing the method of solution in a case of practical interest and not requiring high accuracy.

E. W. C.

**1148.** ALSTON S. HOUSEHOLDER, "Generation of errors in digital computations," Amer. Math. Soc., *Bulletin*, v. 60, 1954, p. 234–247.

This paper is an address delivered before the Spartanburg meeting of the Society on November 28, 1953.

The problem of computing the numerical values of $f(x)$ is considered. In general one must use, in the computation, an approximation $x^*$ to $x$, and an approximation $f_a(x^*)$ to the function $f(x^*)$. The error is expressed as a sum of three independent components: $f(x) - f(x^*)$, $f(x^*) - f_a(x^*)$ and $f_a(x^*) - f^*(x^*)$, called, respectively, the propagated error, the residual error and the generated error. The article treats the generated error. It is stated that differences among high-speed computing machinery are such that each machine demands a theory on the generated error. A specific computing system, the ORACLE, is described and the generated error for certain computational sequences is discussed.

E. W. C.

**1149.** L. KNIGHT, "Valve reliability in digital calculating machines," *Electronic Engineering*, January, 1954, p. 9–13.

A survey is presented of some considerations in selecting vacuum tube types, designing circuits to provide useful tolerences for the tubes, testing them, and maintaining vacuum tube equipment in order to achieve a level of reliable operation demanded by digital calculating machines. Special consideration is given to effects that develop as tubes age. Results of some vacuum tube experience with the Hollerith type 541 multiplier and the Manchester University computer are given.

RUSSELL A. KIRSCH

NBSCL

**1150.** T. PEARCEY, *Use of Punched Cards for Fourier Synthesis*. Division of Radiophysics, Commonwealth Scientific and Industrial Research Organization, RPR 121. Melbourne, November 1953, p. 1–20.

The synthesizing of series of orthogonal functions is described in detail for the case of two-dimensional Fourier synthesis. Hand selection and refiling of cards from two master files of about 4000 cards are performed. The master files should allow for adequate spacing of the variables and positive as well as negative coefficients. The accuracy obtainable by the described method is three digits. The only equipment necessary is a tabulator for summing, a sorter and possibly a collator.

STANLEY PRUSCH

NBSCL

**1151.** R. M. SAUNDERS, "Digital computers as an aid in electric machine design," *Communications & Electronics*, May 1954, p. 189.

An S.O.S. from Industry to the Electronic Brain to take over the drudgery of re-iterative computations required for designing electric machines.

There are tables showing the variables in the design of synchronous machines and a table of operations and sample calculations for ascertaining performance of a ½-hp. induction motor. The "digital approach" and its advantage over hand computations is discussed.

Discussion, pro and con, by ROBERT L. FILLMORE and C. G. VEINOTT is followed with a rebuttal by Saunders.

A. R. COCK

NBSCL

## NEWS

**Numerical Analysis Research, UCLA.**—Numerical Analysis Research, UCLA, is continuing much of the research program of the Institute for Numerical Analysis (INA) of the National Bureau of Standards; INA was disbanded on 30 June 1954 [*MTAC*, v. 8, p. 178].

The new organization, administered by the UCLA Mathematics Department, will receive support from the Office of Naval Research and the Office of Ordnance Research. Its primary mission includes pertinent fundamental research in mathematics and science and research in the application of computers to problems occurring in science and other applied fields. It will be aided in attaining these objectives by the use of the National Bureau of Standards Western Automatic Computer (SWAC) and other equipment which has been loaned to UCLA. In addition, the new organization has the use of INA's library. Most of the research staff of INA has joined the new organization.

The organization offers a training program in the efficient application of high-speed digital computers. A number of graduate assistantships offered in cooperation with various university departments are available each year. Seminars, and formal and informal courses in numerical analysis are conducted.

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## OTHER AIDS TO COMPUTATION

# A Useful Technique in Programming for Analog Computers

In programming for analog computers programmers have found certain types of linear differential equations difficult to handle even with the use of arbitrary function generators. In this paper a technique is presented which enables the analog computer to solve a heretofore difficult set of problems. The technique, while most useful in linear problems, is also useful in other problems. In many cases the technique will reduce the sensitivity of the solution to noise.

Let us consider the general ordinary differential equation

$$f(y,y',y'',\cdots,x) = 0 \tag{1}$$

with the parametric transformation

$$\phi(x,\dot{x},\ddot{x},\cdots,t) = 0. \tag{2}$$

One sets up feedback circuits to generate $x$ and functions of $x$ and uses these to generate $y$. In the case $\phi = x - t = 0$ one gets the usual setup. The special case $\phi = x \pm e^{at} = 0$ has several advantages in certain cases. Two examples following show its use:

Consider the equation

$$(2x^{\frac{1}{2}} + x)y' + (3x^{-.1} + x^{-10})y = 2x^{.45}. \tag{3}$$

For $x > 1$, let $x = e^t$. Then one gets

$$\dot{y} = [2e^{.45t} - y(3e^{-.1t} + e^{-10t})]/(1 + 2e^{-t/2}) \tag{4}$$

which is easy to set up, generating the exponentials in individual integrator-pot-amplifier loops. Of course, one plots $y$ against $e^t$, not $t$.

An example for which this technique is useful in a non-linear equation is the following:

$$Ay'' + By' + Cy^{\frac{1}{2}}e^{-D/y} = 0. \tag{5}$$

Let $v = dy/dx$ and let $y = e^t$. Then $dx/dt = e^t/v$ and thus (5) becomes

$$\dot{v} = \alpha e^t + \beta v^{-1} \exp\left(\tfrac{3}{2}t - De^{-t}\right), \tag{6}$$

where

$$\alpha = -B/A, \quad \beta = -C/A,$$

which can be generated without the use of special function generators.

A parametric substitution as in the above examples can frequently eliminate or considerably reduce the need for special function generators. Other parameterizations can be used, but that which is best can only be determined by an investigation of the specific problem under consideration.

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## BIBLIOGRAPHY Z

1152. S. AMITSUR, U. OPPENHEIM & A. MANY, "An electrical computer for the solution of linear simultaneous equations," *Rev. Sci. Instruments*, v. 24, 1953, p. 112–116.

A variation of the Many-Meiboom network[1] is given which will solve a symmetrical system of linear equations. The given system of equations is analogous to the statement of Kirchhoff's laws for a circuit of pure reactances. Transformers permit the representation of negative nondiagonal quantities by condensers but diagonal negative quantities necessitate the use of coils. The problem of phase difference between the input and output alternating voltages is discussed in detail.

F. J. M.

[1] A. MANY & S. MEIBOOM, "An electrical network for determining the eigenvalues and eigenvectors of a real symmetric matrix," *Rev. Sci. Instruments*, v. 18, 1947, p. 831–836.

**1153.** V. C. ANDERSON & PHILIP RUDNICK, "A thermistor bridge correlator," *Rev. Sci. Instruments*, v. 24, 1953, p. 360–361.

Thermistors are used to obtain the squares of voltages for use in a quarter square multiplier.

F. J. M.

**1154.** N. F. BARBER, "Harmonic analysis," *Rev. Sci. Instruments*, v. 24, 1953, p. 329.

An improvement in the method of F. B. DANIELS[1] is suggested.

[1] F. B. DANIELS, "A planimetric method of harmonic analysis," *Rev. Sci. Instruments*, v. 23, 1952, p. 369–370; *MTAC*, v. 7, p. 120.

**1155.** M. L. BOAS, "Nomograms used in analysis of data in the reaction $Li^6(n,\alpha)H^3$," *Rev. Sci. Instruments*, v. 24, 1953, p. 356–359.

**1156.** S. L. BROWN & H. D. SCHWETMAN, "The application of the Laplace transformation and a mechanical harmonic synthesizer in the analysis of electric circuits," *Rev. Sci. Instruments*, v. 24, 1953, p. 375–379.

The harmonic synthesizer is a purely mechanical one, using gear ratios, scotch yokes and a chain adder. The harmonic synthesizer is used to plot the values of $P(z)$ on a circle $|z| = r$. Thus the real part of $P(z)$ is given by $\sum_{k=0}^{n} a_k r^k \cos k\varphi$ and the imaginary part by a similar expression. The synthesizer is used to plot the complex number $P(z)$ and the number of times this graph loops the origin is the number of roots of $P(z)$ within the circle. Two examples are given with detailed references to specific circuits.

F. J. M.

**1157.** G. L. BROWNELL, R. V. CAVICCHI & K. E. PERRY, "An electrical analog for analysis of compartmental biological systems," *Rev. Sci. Instruments*, v. 24, 1953, p. 704–710.

An analogy is set up between a biological system consisting of fluids in various compartments and an electrical circuit consisting of condensers connected by resistors. The condensers receive an initial charge at intervals of a tenth of a second and the transient response of the system is indicated on an oscilloscope. The system is used to analyze the results of tracer experiments. Models or simply diffusion constant values are hypothecated and tested by the analyzer and the results compared with experimental values obtained by the use of traces of radioactive elements.

F. J. M.

**1158.** A. B. CAMBEL & PAUL J. SCHNEIDER, "Membrane apparatus for analogic experiments," *Rev. Sci. Instruments*, v. 24, 1953, p. 513–514.

A soap film apparatus for solving the Laplacian equation is described.

**1159.** I. CEDERBAUM, "Note on high speed product integrator," *Rev. Sci. Instruments*, v. 24, 1953, p. 1072–1073.

The author obtains an exact expression for the error due to the variation of $y$ in the Macnee set up described in MACNEE (**1163**) in the case in which

the kernel $K$ is trigonometric and $y$ varies either continuously or in small discrete steps.

F. J. M.

**1160.** C. B. CRUMB, JR., "Engineering uses of analog computing machines," *Mechanical Engineering*, v. 74, 1952, p. 635–639.

This is an introductory article which points out the nature of differential analyzers, both mechanical and electrical, various possible applications and a brief description of how such a computer is used.

F. J. M.

**1161.** C. A. LUDEKE & R. T. EVANS, "A coupling analog for nonlinear systems with more than one degree of freedom," *Jn. Appl. Physics*, v. 24, 1953, p. 119–122.

C. A. LUDEKE & C. L. MORRISON, "Analog computer elements for solving nonlinear differential equations," *Jn. Appl. Physics*, v. 24, 1953, p. 243–248.

The objective of the work of these papers is to develop a differential analyzer, whose elementary component contains a representation of a nonlinear differential equation of the second order, for instance

$$\frac{d^2\theta}{dt^2} + f(\theta) = 0.$$

In the second paper, which seems to precede the first logically, such an element is developed in the form of a coil suspended as a pendulum within another coil. The angle of rotation of the coil is the dependent variable and it can be used in turn to rotate a mask controlling the amount of light which falls on a photo tube. The output of the latter is amplified and the resulting current passes through the coil on the pendulum. This yields a possible representation of $f(\theta)$ as a restoring force dependent upon the dependent variable, $\theta$. A number of examples of periodic motions are quoted and good accuracy in the frequency is indicated. In the first paper, coupling between two such units by mounting two coils on each pendulum is described.

F. J. M.

**1162.** F. J. MCDONAL, "A Fourier analyzer," *Rev. Sci. Instruments*, v. 24, 1953, p. 272–276.

This instrument was developed to provide frequency analysis of transient signals, obtained on a multichannel recorder with band width of 5 to 200 cps, during seismic prospecting for oil. The record on variable area film is read by a photoelectric cell, and thus the function to be transformed is obtained as a voltage. A scotch yoke produces the sines and cosines in a form which yields a shaft rotation and hence a linear potentiometer can be used as a multiplier. Integration is by a tachometer type servo integrator and the output appears on a revolutions counter.

F. J. M.

**1163.** A. B. MACNEE, "A high speed product integrator," *Rev. Sci. Instruments*, v. 24, 1953, p. 207–211.

The integrals

$$F(y) = \int_0^T f(t)K(y,t)dt \quad \text{or} \quad \int_0^y f(t)K(y,t)dt$$

are evaluated by means of high speed analog computer elements for various values of $y$. The variable $y$ is given a sequence of values and by a suitable switching procedure the values of $F(y)$ are evaluated at a rate of 60 per second and plotted with a reference value on a cathode ray tube. The functions $f(t)$ and $K(y,t)$ for $y$ fixed are obtained by function generators or by differential analyzer techniques. During the generation of $F(y)$, $y$ which should remain fixed does actually vary. The error due to this cause and the errors due to the multiplier and function generator are discussed.

F. J. M.

**1164.** J. R. RAGAZZINI & G. REYNOLDS, "The electronic complex plane scanner," *Rev. Sci. Instruments*, v. 24, 1953, p. 523–527.

A rational function $F(z)$ is supposed given in the form of a quotient of products of linear factors $z - \lambda_i$. It is required to obtain $\log |F(jw)|$ and $\arg F(jw)$ where $j = \sqrt{-1}$ and $w$ is real. $\text{Log } |F(jw)|$ is the sum of $\pm \log |(jw - \lambda_i)|$. The quantity $jw - \lambda_i$ is represented as a complex voltage and $\log |(jw - \lambda_i)|$ is obtained by a suitable circuit. The argument of $F(jw)$ is obtained by differentiation using the Cauchy-Riemann equations.

F. J. M.

**1165.** J. TADAYON, "Measurement of the angle between two curves," *Rev. Sci. Instruments*, v. 24, 1953, p. 871–872.

An optical instrument for measuring the angle between two curves on a graph is based on the mirror principle for finding the normal to a curve.

F. J. M.

## NOTES

**168.**—A PRACTICAL REFUTATION OF THE ITERATION METHOD FOR THE ALGEBRAIC EIGENPROBLEM. In the second part of my paper on algebraic eigenproblems[2] I have proved that the computation by means of the formation of the characteristic equation requires less computational work than the iteration method, and that this holds even when nothing but the first eigenvalue has to be calculated. This advantage grows with every accessory eigenvalue or vector. Further one has no trouble with deflation which requires a lot of multiplications. Also one can compute every eigenvalue and vector apart from the others, and do this to any desired accuracy, by the more powerful methods for algebraic equations. At last, there arise no difficulties from an unfavorable quotient of the two dominant eigenvalues.

The reason these facts are not yet universally acknowledged is that the iteration method seems to be simpler and more mechanical in its application. But one has to consider that iteration does not converge quickly enough in practice, unless the quotient of the two dominant eigenvalues is $\frac{1}{4}$ or less. This last will be rarely the case. For the eigenvalues must lie somewhere between two circles around the origin in the complex plane. The radius of

the inner circle has a value quite different from zero (if the determinant of the matrix is $\neq 0$). In this ring can lie only some of the $n$ eigenvalues having a quotient less than $\frac{1}{4}$. The other eigenvalues must cluster around some circles. In proportion as the situation is more favourable for e.g. the two dominant eigenvalues, the smaller the room will be for the other ones. There is no escape from this situation, and sooner or later the then dominant eigenvalues will lie close together.

That iteration may give trouble in the most simple cases is a well known fact from numerous calculations. Yet the following example of a symmetric $4 \times 4$ matrix, the eigenproblem of which is therefore real, is amazing.

$$A = \begin{vmatrix} 2 & 1 & 3 & 4 \\ 1 & -3 & 1 & 5 \\ 3 & 1 & 6 & -2 \\ 4 & 5 & -2 & -1 \end{vmatrix}$$

Let $\mu$ be the dominant eigenvalue. Following AITKEN,[1] we begin the iteration with the usual starting vector $v = (1,1,1,1)'$ and so compute $v_m = Av_{m-1}$. The quotient $\mu_m$ of the first components of $v_m$ and $v_{m-1}$ yields for $\mu$ the "approximations":

$$S: \quad \mu_2 = 7.2,\ \mu_3 = 7.5,\ \mu_4 = 7.85,\ \mu_5 = 7.56,\ \mu_6 = 8.0,\ \mu_7 = 7.6,$$
$$\mu_8 = 8.08,\ \mu_9 = 7.667,\ \mu_{10} = 8.122,\ \mu_{11} = 7.683.$$

The convergence is not impressive, especially if one considers that the sequence $S$ converges to about $-8$ (minus eight)! On the contrary, $S$ seems to diverge or to "converge" to two limits.

To analyze the sequence $S$ more deeply, all eigenvalues and vectors were computed from the characteristic equation, the vectors by the method described in BODEWIG,[2] part II, section 3, p. 1–3. These are to 8D

$$\mu^{(1)} = -8.02857835,\ \mu^{(2)} = 7.93290472,\ \mu^{(3)} = 5.66886436,\ \mu^{(4)} = -1.57319074.$$
$$x^{(1)} = (1,\ 2.50146030,\ -0.75773064,\ -2.56421169)'$$
$$x^{(2)} = (1,\ 0.37781815,\ 1.38662122,\ 0.34880573)'$$
$$x^{(3)} = (1,\ 0.95700152,\ -1.42046826,\ 1.74331693)'$$
$$x^{(4)} = (1,\ -0.90709211,\ -0.37759122,\ -0.38331238)'.$$

Since $S$ does converge to $-8.0\ldots$ the situation seems to be that the $\mu_i$ diverge in the beginning. The $\mu_{2i}$ decrease and the $\mu_{2i+1}$ increase, and in order to converge to $-8$, the $\mu_{2i}$ go through zero and the $\mu_{2i+1}$ through $\infty$. By a special method the index has been determined where the signs change. This is the case at the 363rd or 364th iteration.

To demonstrate this conclusion we have computed the values of $\mu_i$ which would have resulted if the iterations had been really effected. The 100th to 102nd iteration would yield the "approximations":

$$\mu_{100} = 7.28514, \quad \mu_{101} = 8.64677.$$

The 200th to 202nd iteration would yield:

$$\mu_{200} = 5.96936, \quad \mu_{201} = 10.57380.$$

The 300th to 302nd would be:

$$\mu_{300} = 2.86532, \quad \mu_{301} = 22.13220.$$

Our above conjecture concerning the $\mu_{2i}$ and $\mu_{2i+1}$ is therefore confirmed, as is also apparent from theoretical reasons. Near the critical point 363 we should get

$$\mu_{360} = 0.13587, \mu_{361} = 468.66407, \mu_{362} = 0.04022, \mu_{363} = 1583.336,$$
$$\mu_{364} = -0.055448, \mu_{365} = -1148.735.$$

The 400th to 402nd iteration would give

$$\mu_{400} = -1.75101, \quad \mu_{401} = -36.46902,$$

the 800th to 802nd:

$$\mu_{800} = -7.94348. \quad \mu_{801} - 8.11356,$$

and at last the 1200th to 1202nd:

$$\mu_{1200} = -8.02787279, \quad \mu_{1201} = -8.02927758.$$

Thus 1200 iterations will scarcely yield 4 figures of the dominant eigenvalue! And this for a simple matrix of order 4.

This amazing conduct can afterwards be explained from the knowledge of the eigenvalues and vectors. The slow convergence has two sources. Not only have the dominant eigenvalues nearly the same absolute value, but also the starting vector $v$ is nearly orthogonal to $x^{(1)}$. In fact writing $x^{(1)}$ in the approximate form $(4,10,-3,-10)'$, the cosine between $v$ and $x^{(1)}$ is only $1/30$ which is about cos 88°.

Yet the situation would not considerably improve if another starting vector, e.g. $(1,0,0,0)'$ would be taken. Nor should we waste time by computing the eigenproblem of matrices of the form $A + c$ with varying $c$'s. The time is better spent by computing the characteristic equation as is pointed out in BODEWIG[2] (Part II in "Zusammenfassung"). Even the use of quadratic equations would not be very efficient in our case as $\mu^{(3)}$ lies close to $\mu^{(2)}$. Nor would this be the case for other matrices if one wants to have more than the two dominant eigenvalues, and even then the determination of the vectors is far from agreeable.

We owe to VON MISES[3] the discovery of the iteration method for finding the dominant value and vector and to AITKEN its application to all complicated cases more or less, and to HOTELLING the discovery of deflation. But times have changed. In our days also the higher eigenvalues and vectors must be computed and with extra accuracy. A deeper analysis shows that the iteration method in its present form is not appropriate and that even in cases when, by exception, the first eigenvalue is furnished quickly the later eigenvalues present the greater troubles.

So the whole eigenproblem must be considered anew.

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[1] A. C. AITKEN, "The evaluation of the latent roots and latent vectors of a matrix," Roy. Soc. Edinburgh, *Proc.*, v. 57, 1936–1937, p. 269–304.
[2] E. BODEWIG, "Bericht über die Methoden zur numerischen Lösung algebraischer Eigenwertprobleme," Seminario matematico e fisico dell' Universita di Modena, *Atti*, v. 4, 1949–1950, v. 5, 1950–1951.
[3] R. VON MISES, "Praktische Methoden zur Gleichungsauflösung," *Zeit. angw. Math. Mech.*, v. 9, 1929, p. 62–77.

**169.**—ANALYTICAL APPROXIMATIONS. [See also NOTE **157.**] The following are approximations for the exponential integral and certain Bessel functions.

(56) $0 \leq x \leq 1 \quad |\epsilon|_{\max} = 2 \times 10^{-7}$

$$-\mathrm{Ei}(-x) + \log_e x \doteq -.57721566 + .99999193\,x - .24991055\,x^2 + .05519968\,x^3 - .00976004\,x^4 + .00107857\,x^5$$

(57) $-3 \leq x \leq 3 \quad |\epsilon|_{\max} = 10^{-7}$

$$J_0(x) \doteq 1 - 2.2499997\,(x/3)^2 + 1.2656208\,(x/3)^4 - .3163866\,(x/3)^6 + .0444479\,(x/3)^8 - .0039444\,(x/3)^{10} + .0002100\,(x/3)^{12}$$

(58) $0 \leq x \leq 3 \quad |\epsilon|_{\max} = 2 \times 10^{-8}$

$$Y_0(x) - \frac{2}{\pi}\log_e\frac{x}{2}\,J_0(x) \doteq .36746691 + .60559366\,(x/3)^2 - .74350384\,(x/3)^4 + .25300117\,(x/3)^6 - .04261214\,(x/3)^8 + .00427916\,(x/3)^{10} - .00024846\,(x/3)^{12}$$

(59, 60) $3 \leq x < \infty$

$$J_0(x) = x^{-\frac{1}{2}} f_0(3/x) \cos\{x - \varphi_0(3/x)\}$$
$$Y_0(x) = x^{-\frac{1}{2}} f_0(3/x) \sin\{x - \varphi_0(3/x)\}$$
$$|\epsilon|_{\max} = 10^{-8}$$
$$f_0(3/x) \doteq .79788456 - .00000077\,(3/x) - .00552740\,(3/x)^2 - .00009512\,(3/x)^3 + .00137237\,(3/x)^4 - .00072805\,(3/x)^5 + .00014476\,(3/x)^6$$
$$|\epsilon|_{\max} = 5 \times 10^{-8}$$
$$\varphi_0(3/x) \doteq .78539816 + .04166397\,(3/x) + .00003954\,(3/x)^2 - .00262573\,(3/x)^3 + .00054125\,(3/x)^4 + .00029333\,(3/x)^5 - .00013558\,(3/x)^6$$

(61) $0 \leq x \leq 3 \quad |\epsilon|_{\max} = 5 \times 10^{-9}$

$$J_1(x)/x \doteq .5 - .56249985\,(x/3)^2 + .21093573\,(x/3)^4 - .03954289\,(x/3)^6 + .00443319\,(x/3)^8 - .00031761\,(x/3)^{10} + .00001109\,(x/3)^{12}$$

(62) $0 \leq x \leq 3 \quad |\epsilon|_{\max} = 5 \times 10^{-8}$

$$\left\{Y_1(x) - \frac{2}{\pi}\log_e\frac{x}{2}\,J_1(x)\right\}x \doteq -.6366198 + .2212091\,(x/3)^2 + 2.1682709\,(x/3)^4 - 1.3164827\,(x/3)^6 + .3123951\,(x/3)^8 - .0400976\,(x/3)^{10} + .0027873\,(x/3)^{12}$$

(63, 64) $3 \leq x < \infty$

$$J_1(x) = x^{-\frac{1}{2}} f_1(3/x) \sin\{x - \varphi_1(3/x)\}$$
$$Y_1(x) = -x^{-\frac{1}{2}} f_1(3/x) \cos\{x - \varphi_1(3/x)\}$$
$$|\epsilon|_{\max} = 3 \times 10^{-8}$$

$$f_1(3/x) \doteq .79788456 + .00000156\,(3/x) + .01659667\,(3/x)^2 + .00017105\,(3/x)^3 - .00249511\,(3/x)^4 + .00113653\,(3/x)^5 - .00020033\,(3/x)^6$$

$$|\epsilon|_{\max} = 8 \times 10^{-8}$$

$$\varphi_1(3/x) \doteq .78539816 - .12499612\,(3/x) - .00005650\,(3/x)^2 + .00637879\,(3/x)^3 - .00074348\,(3/x)^4 - .00079824\,(3/x)^5 + .00029166\,(3/x)^6$$

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170.—A Sieve Problem on "Pseudo-squares." The following problem originated by Kraitchik,[1] and extended by Lehmer[2] by a special sieve, has recently been further extended by the SWAC. Let $p$ be a prime. Let $N_p$ be the least positive non-square integer of the form $8x + 1$ that is a quadratic residue of all primes $\leqslant p$. In this definition, zero is not counted as a quadratic residue so that $N_p$ is not allowed to be divisible by any primes $\leqslant p$. Since squares are quadratic residues of any prime, the numbers $N_p$ behave like squares and may be called pseudo-squares. This fact makes the problem of discovering pseudo-squares not only a sifting problem but also one of rejecting squares. Thus the problem is unsuitable for a high speed sieve alone since the output would be mostly squares, each of which would have to be tested by a more elaborate arithmetic unit. The problem is therefore one for an all-purpose computer programmed for sifting.[3]

Since for $p > 3$, $N_p$ must be of the form $24x + 1$. One may proceed to exclude values of $x$ using prime moduli between 5 and $p$ inclusive. For every value of $x$ not excluded the machine is programmed to extract the square root of $24x + 1$. If this is a perfect square, the machine returns to the sifting program for the next value of $x$. Fortunately the early part of the program, where the squares come thick and fast, had already been carried[2] as far as $N_{61} = 48473881$ in 1928 so that when programmed for the SWAC the routine spends most of its time sifting. Actually, for the record, the SWAC was instructed to print out every 64th square it produced. The complete table of $N_p$ for $p < 83$ is as follows.

| $p$ | $N_p$ | $p$ | $N_p$ | $p$ | $N_p$ |
|---|---|---|---|---|---|
| 2 | 17 | 19 | 53881 | 47 | 9257329 |
| 3 | 73 | 23 | 87481 | 53 | 22000801 |
| 5 | 241 | 29 | 117049 | 59 | 48473881 |
| 7 | 1009 | 31 | 515761 | 61 | 48473881 |
| 11 | 2641 | 37 | 1083289 | 67 | 175244281 |
| 13 | 8089 | 41 | 3206641 | 71 | 427733329 |
| 17 | 18001 | 43 | 3818929 | 73 | 427733329 |
| | | | | 79 | 898716289 |

All $N_p$ above are primes except for

$$N_{11} = 19 \cdot 139$$
$$N_{17} = 47 \cdot 383$$
$$N_{29} = 67 \cdot 1747$$
$$N_{41} = 643 \cdot 4987$$

The interest in pseudo-squares is heightened by the fact that they may be used in tests for primality, as shown by MARSHALL HALL.[4] The operation of the SWAC and the reduction and checking of the output data was done by JOHN SELFRIDGE.

D. H. L.

[1] M. KRAITCHIK, *Recherches sur la Theorie de Nombres*, v. 1, Paris, 1924, p. 41–46.
[2] D. H. LEHMER, "The mechanical combination of linear forms," *Amer. Math. Monthly*, v. 35, 1928, p. 114–121.
[3] D. H. LEHMER, "The sieve problem for all-purpose computers," *MTAC*, v. 7, 1953, p. 6–14.
[4] M. HALL, "Quadratic residues in factorization," Amer. Math. Soc., *Bull.*, v. 39, 1933, p. 578–763.

**171.**—L. F. RICHARDSON (1881–1953). This English mathematician made several notable contributions to numerical analysis. A brief account of his life by P. A. SHEPPARD appears in *Nature* (v. 172, 1953, p. 1127–8).

His work on numerical analysis (apart from that appearing incidentally in his book[1]) was mainly contained in three long papers:

A: "The approximate arithmetical solution by finite differences of physical problems, involving differential equations with an application to the stresses in a masonry dam." Royal. Soc. *Phil. Trans.*, v. 210 A, 1910, p. 307–357.

B: "The deferred approach to the limit"—Part I, L. F. RICHARDSON, Part II, J. A. GAUNT, Royal Soc. *Phil. Trans.*, v. 226 A, 1926, p. 299–361.

C: "A purification method for computing the latent columns of numerical matrices and some integrals of differential equations," Royal Soc. *Phil. Trans.*, v. 242 A, 1950, p. 439–491.

There were minor contributions in

D: "Theory of the measurement of wind by shooting spheres upward," Royal Soc. *Phil. Trans.*, v. 223 A, 1923, p. 345–361.

An introduction to some of the material of A, B appeared in

E: "How to solve differential equations approximately by arithmetic," *Math. Gazette* v. 12, 1925, p. 415–421.

and one to some of the material of C in

F: "A method for computing principal axes," *British Jn. of Psychology*, v. 3, 1950, p. 16–20.

His work is highly individualistic and his language and symbolism picturesque. For instance he introduced the terms "marching" problem, for initial value problems of the form

$$y'' = ky, \quad y(0), \quad y'(0) \text{ given},$$

and "jury" problem for a problem of the form

$$y^{vi} - 3y^{iv} + 3y'' - y = \lambda y, \; y = y'' = y''' = 0 \text{ for } x = \pm 1.$$

We shall discuss briefly two of Richardson's contributions to numerical analysis.

Richardson early in his life recognized the importance of the use of central difference operators in numerical applications, a fact which had been pointed out somewhat earlier by W. F. SHEPPARD. The use of central-difference approximation to derivatives suggested that the (local) difference between the solution to a discrete problem and that of the continuous problem would be a power series in $h^2$, $h$ being the mesh-length. Taking account of the first term only, it is possible by solving the discrete problem for two values of $h$, and then eliminating the $h^2$-contribution to obtain a better approximate solution. This he called the "deferred approach to the limit." Among his examples were the extrapolation from the perimeter of a square and hexagon to that of a circle (see *MTAC* v. 2 1946, p. 114 and p. 223–4) and the evaluation of $e$. He also indicated the passage to the fundamental frequency of a continuous string from that of strings of beads. Richardson is mainly concerned with applications of his method to the numerical solution of differential equations; there are, however, discussions in D of a quadrature and the solution of a Volterra type integral equation.

In B he examines in some detail the justification of this process, considering two main questions: (1) Are the odd-powers of $h$ always absent? (2) How small must $h$ be in order that $h^2$-extrapolation may make an improvement? We shall not discuss this paper in detail: Undoubtedly the process is a valuable practical tool, but there are certainly cases where it is unreliable.[2] Richardson was fully aware of the possible failures and difficulties which might be encountered in its application and discussed various bad examples.

The latter part of A is concerned with a detailed study of the stresses in a dam, with particular reference to a model of the Assuan dam.

An interesting remark in A concerns the cost of computation about 1910. The unit operation was the evaluation of

$$v_N + v_W + v_S + v_E - 4v_0$$

and for this the rate was $n/18$ pence where $n$ was the number of digits carried. An average output in the case $n = 3$ was of the order of 2,000 *correct* units per week, paying about 28 shillings or about 5 dollars at the then current rate.

The second contribution of Richardson which we shall discuss is an algorithm for the solution of a system of $n$ linear equations, $A\mathbf{x} = \mathbf{b}$. This is to choose an arbitrary $\mathbf{x}^{(0)} = \{x_i^{(0)}\}$ and then put

$$\mathbf{x}^{(r+1)} = \mathbf{x}^{(r)} + \beta_r\{A\mathbf{x}^{(r)} - \mathbf{b}\},$$

where the factors $\beta_r$ are to be chosen. Some suggestions for their choice was given in A; an up-to-date study has been given by D. M. YOUNG.[3]

The success of this algorithm can be established by expressing the errors in terms of the characteristic values of $A$. Following Young we assume that $A$ has linearly independent characteristic vectors $\mathbf{v}_1, \cdots, \mathbf{v}_n$ with characteristic values $\lambda_1, \cdots, \lambda_n$. Then the error vector $\boldsymbol{\varepsilon}^{(r)} = \mathbf{x}^{(r)} - \mathbf{x}$ satisfies

$$\boldsymbol{\varepsilon}^{(r+1)} = \boldsymbol{\varepsilon}^{(r)} + \beta_r A\boldsymbol{\varepsilon}^{(r)}.$$

If we expand $\epsilon^{(0)}$ in terms of the $\mathbf{v}_i$ as: $\epsilon^{(0)} = \sum_{i=1}^{n} c_i \mathbf{v}_i$ we find

$$\epsilon^{(r)} = \sum_{i=1}^{n} c_i \mathbf{v}_i \prod_{k=1}^{r} (1 + \beta_k \lambda_i).$$

This gives

$$\|\epsilon^{(r)}\|^2 = \sum_{i=1}^{n} c_i^2 \|\mathbf{v}_i\|^2 \left\{ \prod_{k=1}^{r} (1 + \beta_k \lambda_i)^2 \right\} \leqslant \|\epsilon^{(0)}\|^2 M^{(r)}$$

where

$$M^{(r)} = \max_{1 \leq i \leq n} \left\{ \prod_{k=1}^{r} (1 + \beta_k \lambda_i)^2 \right\}.$$

For convergence we have to show that $M^{(r)} \to 0$. In practice the sequence of $\beta_r$ will often be taken as periodic and then it will be sufficient if the product taken over a period, is less than unity. In this case, if we know, for instance, that

$$0 < \lambda_r \leqslant b, \quad r = 1,2,\cdots,n$$

and choose $\beta_r$ so that $0 > \beta_r > -2b^{-1}$, then each factor will be less than unity and convergence is assured.

It is clear that these ideas can also be used in the practical determination of the characteristic vectors of a matrix. Suppose we have an approximation $\mathbf{v}$ to a characteristic vector $\mathbf{v}_1$ of a matrix $A$ and, for simplicity, assume that the only contamination is a component of the characteristic vector $\mathbf{v}_2$. Suppose we have $\mathbf{v} = c_1\mathbf{v}_1 + c_2\mathbf{v}_2$. Let $\lambda_1,\lambda_2$ be the characteristic values corresponding to $\mathbf{v}_1,\mathbf{v}_2$. Then, for any $\alpha(\neq\lambda_1)$

$$\begin{aligned} \mathbf{v}^{(1)} &= (A - \alpha I)\mathbf{v} = c_1(\lambda_1 - \alpha)\mathbf{v}_1 + c_2(\lambda_2 - \alpha)\mathbf{v}_2 \\ &= (\lambda_1 - \alpha)[c_1\mathbf{v}_1 + c_2(\lambda_2 - \alpha)(\lambda_1 - \alpha)^{-1}\mathbf{v}_2]. \end{aligned}$$

The strength of the component of $\mathbf{v}_2$ will therefore be reduced if $|(\lambda_2 - \alpha| < |\lambda_1 - \alpha|$, i.e. if $\alpha$ is nearer $\lambda_2$ than $\lambda_1$. If this is so successive repetition of the multiplication $A - \alpha I$ will purify $\mathbf{v}$. This method is a generalization of the familiar "power" method for the determination of the characteristic value of largest absolute value.

In C, Richardson exploits this idea, with a wealth of numerical examples, including cases when the matrix is unsymmetric or has non-linear elementary divisors. He discusses the use of purifiers of the form

$$(A - \alpha_1 I)(A - \alpha_2 I)\cdots(A - \alpha_k I)$$

and the optimal choice of the $\alpha_i$. It is clear that information about the location of the characteristic roots is essential for satisfactory choice of the $\alpha_i$. Richardson makes use of the bounds given by HIRSCH, Rayleigh's quotient, and the comparison of the ratios of corresponding components of $A\mathbf{v}$ and $\mathbf{v}$. The latter is used in an intuitive way, no mention being made of the result of COLLATZ, that there is always at least one characteristic root between the greatest and least of the ratios of the components.

J. T.

[1] L. F. RICHARDSON, *Weather Prediction by Numerical Processes*. Cambridge, England, 1923. For the following comment on this, I am indebted to G. E. FORSYTHE, "It is a monumental attempt to forecast for six hours, from almost no initial condition, and (I understand) a poor balance of $\Delta t$ and $\Delta x$, $\Delta y$, $\Delta z$. It is superbly written and the author has (in my opinion) the most elegant English style of any mathematical writer of the century. [See p. 219 of this book, or the first page or two of C.] The Preface speaks for itself of the troubles encountered by the author."

[2] Cf. W. WASOW, "Discrete approximations to elliptic differential equations." *Zeit. f. ang. Math. u. Phys.*, v. 5, 1954.

[3] D. M. YOUNG, "On Richardson's method for solving linear equations with positive definite matrices." *Jn. Math. and Physics*, v. 32, 1953, p. 243–255. Experiments on the solution of the Laplace equation by this method, on ORDVAC, have been carried out by D. M. Young, and C. H. WARLICK.

## CORRIGENDA

V. 8, p. 93, l.-3, *for* $12\mu = \mu^3$ *read* $12\mu + \mu^3$.

V. 8, p. 106, l. 8, *for* PEARCY *read* PEARCEY.

V. 8, p. 121, l. 20 *for* $+3(2 + i)$ *read* $-3(2 + i)$.

EDITORIAL NOTE. With this issue of *MTAC* the present Editorial Committee rounds out its fifth year and resigns. It is a pleasure to thank our many contributors, reviewers and referees for their cooperative assistance to the Committee and to *MTAC*. Future editorial correspondence should be addressed to

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